Computer Model for Predicting Detonation Properties of Slurry Explosives

Final Report

by

B.C.-Y. Lu, W.K. Chung and Y. Adachi
Department of Chemical Engineering, University of Ottawa

Work on this project was conducted under the auspices of the Canada Centre for Mineral and Energy Technology, Energy, Mines and Resources, Canada.

DSS FILE NUMBER : 14SU 23440-2-9178
DSS CONTRACT SERIAL NUMBER : OSU82-00356
CANMET PROJECT NUMBER : 220002
CANMET SCIENTIFIC AUTHORITY : Dr. K.K. Feng

DATE: March 1984

This report should be citeyed as Contract Report No.: OSU82-00356

60 pp

JUL 30 1984
MICROMEDIA

TABLE OF CONTENTS

	PAGE
LIST OF TABLES	i,ii
LIST OF FIGURES	iii
SCOPE OF WORK	1
INTRODUCTION	2
TIGER CODE	4
EQUATIONS OF STATE	5
RESULTS AND DISCUSSION	8
SOLID EXPLOSIVES	8
PETN	9
RDX	11
ANFO	11
LIQUID EXPLOSIVES	12
SLURRY EXPLOSIVES	13
VARIATION OF AMOUNT OF CONSTITUENTS	15
EFFECT OF INERT CONSTITUENT	16
RATE EFFICIENCY	16
COMPUTER TIME	17
CONCLUSIONS	17
ACKNOWLEDGEMENT	18
REFERENCES	19
APPENDIX: COMPUTER PROGRAM FOR SUBROUTINE HS1EOS (LANE)	48

LIST OF TABLES

		PAGE
Table 1.	Comparison of calculated and experimental detonation products (moles/kg explosive) for two ANFO mixtures (density = 0.8 gm/cm^3)	21
Table 2.	Comparison of calculated detonation temperatures for two liquid explosives	22
Table 3.	Calculated results for isopropylnitrate (ρ = 1.137 g/cm^3)	23
Table 4.	Elemental compositions of the ammonium nitrate-loaded slurry explosives investigated	24
Table 5.	Comparison of calculated C-J state and detonation products (NO and CO) for ammonium nitrate-loaded slurry explosives	25
Table 6.	The calculated constant volume explosion state for ammonium nitrate-loaded slurry explosives	27
Table 7.	The calculated Hugoniot curve for ammonium nitrate-loaded slurry explosive #2	28
Table 8.	The calculated isolines for ammonium nitrate-loaded slurry explosive #2 at two conditions	28
Table 9.	The calculated Hugoniot curve for ammonium nitrate-loaded slurry explosive #5	29
Table 10.	The calculated isolines for ammonium nitrate-loaded slurry explosive #5 at two conditions	30
Table 11.	The calculated C-J state and detonation products (NO and CO) for ammonium nitrated-loaded slurry explosive #2 with various amount of aluminum	31

PAGE

Table 12. The calculated C-J state and detonation products (NO and CO) for ammonium nitrated-loaded slurry explosive #3 with various amount of $NaNO_3$ 32

Table 13. The calculated C-J state and detonation products (NO and CO) for ammonium nitrate-loaded slurry explosive #10 with various amount of $Ca(NO_3)_2$ 33

Table 14. The calculated C-J state and detonation products (NO and CO) for ammonium nitrate-loaded slurry explosive #10 with various amount of $NaNO_3$ 33

Table 15. The calculated C-J state and detonation products (NO and CO) for ammonium nitrate-loaded slurry explosive #10 with various amount of aluminum 34

Table 16. The calculated C-J state and detonation products (NO and CO) for ammonium nitrate-loaded slurry explosive #10 with silicon replacing aluminum 34

Table 17. The calculated C-J state and detonation products (NO and CO) for ammonium nitrate-loaded slurry explosive #10 with various amount of $NaNO_3$ and $Ca(NO_3)_2$ 35

Table 18. The calculated C-J state and detonation products (NO and CO) for ammonium nitrate-loaded slurry explosive #9 with various amount of inert added 36

LIST OF FIGURES

		PAGE
Figure 1	Comparison of experimental C-J detonation velocities for PETN with calculated values from hard-sphere equations	37
Figure 2	Effect of the adjustable parameter $\underline{\lambda}$	38
Figure 3	Comparison of calculated and experimental C-J detonation velocities for PETN	39
Figure 4	Comparison of calculated and experimental C-J detonation pressures for PETN	40
Figure 5	Comparison of calculated and experimental C-J detonation temperatures for PETN	41
Figure 6	Comparison of calculated detonation temperature for RDX	42
Figure 7	Comparison of calculated detonation pressure for RDX	43
Figure 8	Comparison of calculated detonation velocities for RDX	44
Figure 9	Comparison of calculated temperature for ANFO ρ=0.8 (g/cm^3), AN:NH_4NO_3, FO:$C_{7\ 17}H_{14}$	45
Figure 10	Comparison of calculated pressure for ANFO ρ=0.8 (g/cm^3), AN:NH_4NO_3, FO:$C_{7\ 17}H_{14}$	46
Figure 11	Comparison of calculated detonation velocities for ρ=0.8 (g/cm^3), AN:NH_4NO_3, FO:$C_{7\ 17}H_{14}$	47

SCOPE OF WORK

The work of this contract is part of CANMET's continuing efforts for the development of new regulatory standards for safety certification of explosives.

The goal of this contract is to develop a suitable model for calculating detonation parameters of slurry explosives. There are two problems to be tackled. The main problem is the calculation of conditions in the Chapman-Jouquet detonation wave (the so-called C-J condition). The second problem is the calculation of the properties of the detonation products along the Hugoniot curve and along isolines of slurry explosives.

INTRODUCTION

This report describes the activities and results obtained for the study on "Computer Model for Predicting Detonation Properties of Slurry Explosives" during the period from January, 1983 to March 1984.

The two requirements of the contracts are:

1. To develop a model for predicting the detonation properties of slurry explosives by using TIGER CODE to enhance the understanding of the behavior of non-ideal explosives.
2. To acquire necessary thermodynamic data for different slurry explosives for calculating properties such as C-J state, Hugoniot curve, constant volume explosion point, points at specified conditions, as well as a grid of points and isolines.

In order to fulfill the goal of the contract, as outlined in the "Scope of Work" section, the following sequence of study has been carried out in this work:

1. Evaluate equations of state (EOS) used in the determination of the C-J condition. Proposed or suggest a suitable EOS, in conjunction with the application of the TIGER CODE, that can reasonably represent ammonium nitrate-loaded slurry explosives at the C-J condition.
2. Evaluate the rate efficiency of ammonium nitrate in slurry explosive mixtures in terms of the difference between observed and calculated detonation properties.
3. Evaluate the effects of inert constituents in the range of 1 to 10% by mass in explosives on the behavior of non-ideal explosives. Inert constituents such as calcium oxide or carbonate, silica, or sodium oxide should be assessed.

This sequence of study follows the suggestion of "Statement of Work" (Appendix "A" of the contract), a copy of which is attached to this report (Appendix I).

In order to reach the stated goal, it was necessary to evaluate various equations of state, including and in addition to those already available in the digital computer program of the TIGER CODE, used in the calculation of detonation properties with the anticipation that a suitable equation be proposed or suggested for calculating the desired detonation properties of ammonium nitrate-loaded slurry explosives.

In this work, we have investigated a total of nine equations of state and calculated detonation properties for three solid explosives, three liquid explosives and twelve ammonium nitrate-loaded slurry explosives.

TIGER CODE

TIGER is a digital computer program for computing detonation properties of condensed explosives, such as the C-J state, Hugoniot curves, constant volume explosion point, specified and grids of points, and isolines.

For a given explosive with known overall composition together with an appropriate equation of state for representing the reaction products, the TIGER CODE is capable of performing the calculation of the desired detonation properties, provided that the required thermodynamic data are available and included in the program library.

In addtion to the ideal-gas equation, the equations of state incorporated in the TIGER CODE include: the Becker-Kistiakowsky-Wilson (BKW) equation, Jacobs-Cowperthwaite-Zwisler (JCZ 2 and JCZ 3) equations and the BRL-SRI equation. However, the application of the CODE is not limited to these equations. Any suitable equation togeher with its expressions of the derived properties properly introduced into the CODE, can be used to perform the calculations mentioned above.

EQUATIONS OF STATE

In addition to the Becker-Kistiakowsky-Wilson (BKW) [1], JCZ 2 [2], BRL-SRI [3] equations, an attempt was made in this work to test and evaluate several hard-sphere equations of state for detonation calculations.

As attractive forces of molecules in a real gas at high temperature are of less importance, equations of state (EOS) involving only hard-sphere repulsive interactions would provide good approximations. One of such equations, the compressibility form of the Percus-Yevick EOS (PYC) [4,5], was selected by Edwards and Chaiken [6] in 1974 in their detonation calculations for pentaerythritol tetranitrate (PETN) and ammonium nitrate-fuel oil (ANFO) explosives.

The general form of a simple EOS for the hard-sphere repulsive term is given by:

$$P = RT\ \phi(y)/V \tag{1}$$

where $\phi(y)$ is the hard-sphere compressibility factor; P, the pressure; R, the gas constant; T, the absolute temperature; and V, the molar volume. The accurate virial expansion of $\phi(y)$, based on the work of Ree and Hoover [7] is given by:

$$\phi(y) = 1 + 4y + 10y^2 + 18.365y^3 + 28.24y^4 + 39.4y^5 + \ldots \tag{2}$$

The quantity y is a density variable. It is defined by:

$$y = \pi\ N_d \sigma^3/6 \tag{3}$$

where N_d is the number density and σ the molecular diameter. The $\phi(y)$ expression for PYC

$$\phi(y) = (1 + y + y^2)/(1 - y)^3 \tag{4}$$

gives the following virial expansion:

$$\phi(y) = 1 + 4y + 10y^2 + 19y^3 + 31y^4 + 46y^5 + \ldots \tag{5}$$

which approximates the coefficients of Eq. 2 very well. On the other hand, the $\phi(y)$ expression proposed by Carnahan and Starling (CS), [8]

$$\phi(y) = (1 + y + y^2 - y^3)/(1 - y)^3 \qquad (6)$$

yields a virial expression

$$\phi(y) = 1 + 4y + 10y^2 + 18y^3 + 28y^4 + 40y^5 + \ldots \qquad (7)$$

which agrees more closely with Eq. 2 than the PYC equation. It appears desirable to evaluate the applicability of the CS equation for detonation calculations.

For the purpose of comparison, three additional expressions of $\phi(y)$ for hard spheres were considered and included in some of the calculations:

Guggenheim [9]	$1/(1 - y)^4$	(8)
Thiele [10]	$(1 + 2y + 3y^2)/(1 - y)^2$	(9)
Scott [11]	$(1 + 2y)/(1 - 2y)$	(10)

In the calculation, the expression for the quantity σ^3 for mixtures adopted by Edwards and Chaiken [6] in their calculations with the PYC equation was followed,

$$\sigma^3 = \lambda \sum_{i=1}^{N} \sum_{j=1}^{N} x_i x_j \sigma_{ij}^3 \qquad (11)$$

where $\sigma_{ij} = (\sigma_i + \sigma_j)/2$; N is the number of species; x_i, the mole fraction of species i; and y, the adjustable parameter.

In this work, Chapman-Jouguet (C-J) detonation calculations were carried out by means of an equation of state together with the existing chemical equilibrium detonation TIGER CODE. The quantities and the derivatives incorporated in the TIGER CODE include the following:

$$\frac{\partial \ln \phi}{\partial \ln T}, \frac{\partial \ln \phi}{\partial \ln \rho}, \frac{\partial \ln \phi}{\partial n_i}, \Gamma_i, \frac{\partial \ln \Gamma_i}{\partial \ln T}, \frac{\partial \ln \Gamma_i}{\partial \ln \rho}, \frac{\partial \ln \Gamma_i}{\partial n_j}, \varepsilon, \varepsilon_T \text{ where}$$

$\rho = Mo/V$

Mo = mass of the system including condensed phases

$$\Gamma_i = \int_0^{\rho} \left[\frac{Mo}{RT\rho} \frac{\partial P}{\partial n_i} - 1\right] \frac{d\rho}{\rho} \qquad (i = 1, \ldots, N)$$

$$\varepsilon = \int_{o}^{\rho} \frac{Mo}{RT\,\rho} \left[P - T \left(\frac{\partial P}{\partial T}\right)\right] \frac{\partial \rho}{\rho}$$

and

$$\varepsilon_T = \int_{o}^{\rho} \left[\frac{Mo\ T}{R\rho} \left(\frac{\partial^2 P}{\partial T^2}\right) \frac{\partial \rho}{\rho}\right.$$

All the necessary mathematical expressions were developed for the hard-sphere equations mentioned above, and included in the computer program.

RESULTS AND DISCUSSION

In this work, detonation properties for the following explosives were obtained:

Solid explosives: PETN, RDX and ANFO

Liquid explosives: Nitroglycerine (NG), Nitromethane (NM) and Isopropylnitrate

Slurry explosives: Twelve ammonium nitrate-loaded slurry explosives

The results obtained from various equations of state were compared with each other and with the available experimental values. The relative performance of these equations was evaluated.

Solid Explosives

The detonation temperatures, pressures and velocities for the three solid explosives were calculated by means of the following equations of state:

BKW, JCZ 2, JCZ 3, BRL-SRI (already incorporated in the TIGER CODE)

BKW with modified parameters (MBKW) [12]

CS, Guggenheim, Thiele, Scott

The values of the parameters originally available in the TIGER CODE and the modified version of the BKW equation of state,

$$\frac{PV}{RT} = 1 + X \exp(\beta X), \quad X = K/[V(T+\theta)^{\alpha}]$$

used in the calculation are listed below:

Equation	α	β	θ	K	Remark
BKW [1]	0.5	0.16	400	10.91	only for RDX
BKW	0.5	0.10	400	11.85	Explosive other than RDX
MBKW [12]	0.5	0.16	1850	8.85	

The values of λ and σ_i reported by Edwards and Chaiken [6] were obtained from a curve fitting method, using the experimental detonation velocities of

Hornig et al. [13] for PETN at 15 charge-loading densities ranging from 0.88 to 1.76 g/cm^3. The range of best λ values was found to be between 0.3350 and 0.4175, and an averaged value of λ = 0.372 was used by these authors. An initial value of λ = 0.35 was arbitrarily selected in the calculation for the purpose of evaluating and comparing the performance of the five hard-sphere equations of state. It should also be mentioned that the values of molecular diameter σ reported by Edwards and Chaiken [6] were adopted in this work without modifications.

PETN

The calculated C-J detonation velocities from the five equations for PETN are shown in Fig. 1. The results indicate that the Scott equation (Eq. 10) yielded the highest values, while the Thiele equation (Eq. 9) yielded the lowest. Furthermore, the values obtained from the CS equation (Eq. 6) are very close to that from the PYC equation (Eq. 4), and the differences are generally less than 2%. The curve obtained from Eq. 9 appears to follow the trend of the experimental values closer than the other equations.

The calculated C-J detonation temperatures and pressures for PETN are practically identical for all equations over the complete range of the loading densities investigated (0.88 to 1.76 gm/cm^3). The maximum deviation observed is about 4%.

It should be mentioned that the location of the curves presented in Fig. 1 depends on the λ values used in the calculation. Various λ values were assumed in the calculations using Eqs. 6 and 9. The results obtained with PETN for the C-J detonation velocity are depicted in Fig. 2. The experimental values reported by Hornig et al. [13], Dremin and Shvedow [14], Fickett [15], Lee and Hornig [16], and Apin and Voskoboynikov [17] together with the curve obtained from the PYC equation with λ = 0.372 [6] are also included in Fig. 2 for comparison.

Although the experimental values cannot be exactly represented by any curve in Fig. 2, which is an indication that the variation of λ values alone is not sufficient to alter the curvature of the curves to fit the data, they can be approximately represented by the CS equation with λ values between 0.35 and 0.40 and by the Thiele equation with slightly higher λ values.

Additional calculations of the C-J detonation velocity, pressure and temperature for PETN were carried out using the BKW, JCZ 2, JCZ 3 and BRL-SRI equations. The parameter values of these equations, other than the BKW equation, were taken from Cowperthwaite and Zwisler [2]. The results obtained are compared with the available experimental values [1, 13-18] and the calculated values obtained from the CS and the PYC equations in Fig. 3-5.

In Fig. 3, the calculated detonation velocities obtained from the JCZ 3 equation are closer to the experimental values in the high density region than all the other equations. The CS equation with $\lambda = 0.40$ and the JCZ 2 equation yield reasonable values in the lower density region.

The detonation pressures obtained for PETN (Fig. 4) from the PYC equation using $\lambda = 0.372$ appeared to be too low in comparison with the experimental values. The CS equation with $\lambda = 0.40$ yielded reasonable detonation pressures in the low density region, but a higher λ value is required to fit the experimental values in the high density region. On the other hand, the BKW equation yielded reasonable detonation pressures in the high density region but not in the low density region.

The detonation temperatures obtained for PETN (Fig. 5) from the hard-sphere and the BRL-SRI equations are closer to the experimental values than those obtained from the BKW, JCZ 2 and JCZ 3 equations. Furthermore, the variation of the calculated detonation temperatures with loading density from the BKW, JCZ 2 and JCZ 3 equations is opposite to that of the experimental values.

It should also be mentioned that the BRL-SRI equation required two to three times more computer time than the hard-sphere equations.

RDX

The detonation temperatures, pressures and velocities for RDX were calculated by means of the BKW, JCZ 3, JCZ 3, BRL-SRI, and CS equations. The results obtained from these equations are presented graphically in Figs. 6-8 in terms of the loading density. The experimental values available in the literature are limited to the detonation temperatures reported by Gibson et al. [18]. It is seen from Fig. 6 that the calculated values obtained from the CS equation (λ = 0.35) are closer to the experimental values than those obtained from the BKW, JCZ 2 and JCZ 3 equations. The differences in the calculated detonation temperatures obtained from the CS and the BRL-SRI equations are not very significant.

ANFO

Further comparison of the performance of the five hard-sphere equations was made using the results obtained with ANFO at a density of 0.8 gm/cm^3 for the C-J detonation velocity, pressure and temperature as a function of the fuel oil percentage. The difference in the calculated values between these equations is less than 3%.

Additional calculations were carried out using the BKW, JCZ 2, JCZ 3 and BRL-SRI equations, and the calculated results are compared with those obtained from the CS equation (λ = 0.35) in Figs. 9-11.

The calculated maximum for the three C-J detonation properties occurred at a fuel content of six percent with all the equations tested, but with different numerical values. The magnitude of the calculated values may be summarized as follows:

Velocity, pressure: BKW JCZ 2 JCZ 3 BRL-SRI, hard-sphere EOS

Temperature: BRL-SRI, hard-sphere EOS JCZ 3 JCZ 2 BKW

The calculated detonation velocities for ANFO indicate that the values from the BKW equation are too high while those obtained from the hard-sphere and the BRL-SRI equations are somewhat lower than the experimental values [19,20].

The detonation products for two ANFO mixtures were calculated using the CS equation with a λ value of 0.35. The calculated values are compared with the calculated results reported by Mohan and Hay [12] in Table 1. The experimental results reported by Chaiken et al. [21] are also included in this table for comparison.

The results indicate that the values obtained from the CS equation agreed very closely with the two sets of observed values, especially the NO product from the second mixture.

Liquid Explosives

For the two liquid explosives, NG and NM, the detonation temperatures calculated from five equations of state (BKW, JCZ 2, JCZ 3, BRL-SRI and CS with λ = 0.35) are compared with the available experimental values in Table 2. It should be mentioned that for NG, the experimental values reported by the U.S. Bureau of Mines and the Los Alamos National Laboratory are different by about 500°C. The values reported by Cook and Mader are also included in Table 2 for comparison. These values were taken from the book by Johansson and Persson [22].

For the liquid explosive NM, the detonation temperature obtained from the CS equation agrees very well with the experimental values. The value obtained from the BRL-SRI equation is slightly higher than the experimental values and is reasonable. The values of Mader and that obtained from the BKW equation appear to be low.

For the liquid explosive NG, the calculated values of detonation temperature by means of the CS and the BRL-SRI equations are higher than the experimental values, but not as high as that of Cook. The values obtained from the JCZ 2 and

JCZ 3 equations appear to be more reasonable. The value obtained from the BKW equation appears to be low.

The calculated C-J detonation temperature, pressure and velocity as well as the detonation gas products NO and CO at the C-J point for liquid explosive isopropylnitrate (loading density = 1.137 g/cm^3) using the CS, BKW and MBKW equations are given in Table 3. Although no experimental values are available for comparison, the results obtained from the BKW equation appear to be less desirable. The calculated detonation temperature is too low and the calculated detonation pressure appears to be too high. On the other hand, the CS and the MBKW equations yielded reasonable values of detonation temperature and predicted the presence of CO in the gas products. It should also be mentioned that it was difficult to obtain calculated values by means of the PYC equation with $\lambda = 0.372$.

Slurry Explosives

In this work, twelve commercially available ammonium nitrate-loaded slurry explosives were investigated. The elemental compositions of these explosives are reported in Table 4.

Four equations of state (CS, PYC, BKW, MBKW) were selected for calculating the C-J conditions and the gas products (NO, CO and total amount of gas in terms of number of moles per kilogram of explosive) for these explosives. The calculated results are reported in Table 5. The experimental values supplied to us are limited to detonation velocities for four slurry explosives:

Slurry explosive	#6	D = 4,000 m/s
" "	#7	D = 4,000 "
" "	#9	D = 3,490 "
" "	#10	D = 4,280 "

The JCZ 2, JCZ 3 and BRL-SRI equations were not used in these calculations due to the lack of parameter values. The BKW and MBKW equations were not used in

the calculation for slurry explosives containing silicon (slurry explosives #11 and 12). The other missing values in Table 5 are due to the difficulties encountered in the calculation. For the slurry explosives #3 and 4, the calculated values from the BKW equation as presented in Table 5 were supplied to us by Dr. K.K. Feng. Identical values were also obtained independently from our own calculations.

The detonation velocity values obtained from the CS equation agree more or less with those obtained from the PYC equation and appear to be in reasonable agreement with the available experimental values. However, calculation difficulties wwere encountered in some of the calculation using the PYC equation with λ = 0.372 as suggested by Edwards and Chaiken [6]. The results obtained from the BKW equation deviate considerable from those obtained from the other three equations.

The detonation pressure values obtained from the two hard-sphere equations (CS and PYC) are lower than those obtained from the BKW and the MBKW equations, and the reverse is true for the calculated detonation temperature values.

The existing data library of the TIGER CODE provided the required thermodynamic data for C, H, N, O, Ca, Na, Al and their various chemical compounds. The thermodynamic data for SiO_2, SiC, Si and $SiCl_4$ were calculated in this work and included in the library for the above calculations.

In view of the good performance of the CS equation, it was selected for the calculation of Hugoniot curves, constant volume explosive points and isolines. Slurry explosives #2 and 5 were selected for these calculation using λ = 0.35. The values obtained are reported in Tables 6-10, indicating the capability of the CS equation for these calculations. In addition, detonation calculations were carried out for a grid of points. Although the numerical values are not reproduced in this report due to the tremendous amount of numbers generated, the results also demonstrated the capability of the CS equation in performing the required calculations.

Variation of Amount of Constituents

In order to study the effect of various amount of constituents in terms of aluminum, silicon and nitrates on the detonation properties, slurry explosives #2, 3 and 10 were selected for the investigation.

The aluminum content in slurry explosive #2 was changed from 1.10% to 10.04% by mass. The calculated C-J state and detonation products in terms of NO and CO are reported in Table 11. The sodium content in terms of $NaNO_3$ in slurry explosive #3 was varied and the calculated results are reported in Table 12. Slurry explosive #10 contains sodium aluminum and calcium. For this explosive, the calculated results are reported in Tables 13-17 as follows:

Table 13 Amount of calcium (in terms of $Ca(NO_3)_2$) varied

Table 14 Amount of sodium (in terms of $NaNO_3$) varied

Table 15 Amount of aluminum varied

Table 16 Aluminum replaced by silicon

Table 17 Total amount of sodium and calcium (in terms of nitrate) kept constant, but relative amounts of the two varied.

The calculated results indicate that in general the values of detonation temperature, pressure, velocity and the amount of CO increase with the increase of the amount of aluminum or silicon. The opposite is true for sodium and calcium. It seems that a maximum exists in the calculated detonation velocities for aluminum (Table 11), but the variation of the values is not significant.

The amount of NO gas product decreased with increasing amount of aluminum or calcium in slurry explosives (Tables 11 amd 13) and increased with increasing amount of sodium (Table 14). When the total amount of sodium and calcium was kept constant (Table 17), very little change was observed in the calculated detonation properties. When the amount of aluminum in slurry exploseve #10 was replaced by silicon, the values of the calculated detonation temperature, pressure

and velocity were actually increased, but can be restored by a decrease of the silicon content (Table 16).

As far as the amount of the toxic gas products (CO + No) is concerned, it seems that a minimum value exists in the case of slurry explosive #2 around 7.25% of aluminum by mass (Table 11). The amount decreased with the increase of sodium for slurry explosive #3 (Table 12) and with the increase of calcium for slurry explosive #10 (Table 13).

It appears to be possible to adjust the amounts of constituents in the commercial slurry explosives to maintain the desired detonation properties and at the same time to minimize the production of toxic gases.

Effect of Inert Constituents

For the purpose of estimating the effect of various amount of inert content on the detonation properties, slurry explosive #9 was selected for the study. Various amounts of Na_2O, CaO, SiO_2 and $CaCO_3$ were added to the explosive, and the calculated C-J state and gas products using the CS equation with $\lambda = 0.35$ are reported in Table 18. The results indicate that, with the exception of Na_2O, an increase in the amount of CaO, SiO_2 or $CaCO_3$ increases the detonation pressure, velocity and temperature. In all cases, an increase of the inert constituent increases the production of NO and CO but reduces the total amount of gas (mols/Kg explosive)

Rate Efficiency

One of the tasks of this study concerns the rate efficiency of ammonium nitrate in slurry explosives in terms of the differences between the observed and calculated detonation properties.

Due to the lack of experimental values, only detonation velocities could be compared. As the calculated values depend on the λ values used in the calculation, they can be made to be identical to the experimental values. Consequently,

it has no real meaning to compare the difference between the experimental values and values obtained from the hard-sphere equations of state studied above. Should it be required to use the hard-sphere equations of state to do the calculation, it would be necessary to establish a correlation between λ and loading density ρ. On the other hand, it was possible to estimate the rate efficiency using the MBKW equation. For example for the slurry explosive #10, the experimental detonation velocity is about 97% of the calculated detonation velocity, while the difference between the experimental and calculated values of detonation velocity being 140 m/sec. This difference is estimated to be equivalent to 13% of the explosive not decomposed.

Computation Time

The time required for the computation depends very much on the possible detonation products included in the consideration. With proper elimination of those unlikely products, it was possible to save the computation time by 90% or even 95%.

CONCLUSIONS

1. The CS equation is capable of producing the desired detonation properties.
2. The adjustable parameter λ is essential in the application of the CS equation. The λ values should be further studies using additional experimental values.
3. It is feasible to maintain the desired detonation temperatue, pressure and detonation velocity; save the cost and minimize the production of toxic gases (NO and CO) by adjusting the amounts of Al, Si, Na and Ca in slurry explosives.
4. Judicial elimination of possible gaseous/condensed detonation products in the calculation could save computation time up to 95%.

ACKNOWLEDGEMENT

The authors wish to express their thanks to Dr. K.K. Feng for his kind assistance throughout this work.

REFERENCES

1. Mader, C.L. "Numerical Modeling of Detonation", University of California Press, 1979.
2. Cowperthwaite, M. and Zwisler, W.H. "The JCZ Equations of State for Detonation Products and Their Incorporation into the TIGER CODE", Proceedings of the Sixth Symposium (International) on Detonation Naval Weapon Center, p. 163, 1976.
3. Cowperthwaite, M. and Zwisler, W.H. "Theoretical and Mathematical Formulation for the TIGER Computer Program", Stanford Research Insitute, California, 1973.
4. Reiss, N.R., Frisch, H.L. and Lebowitz, J.L. "Statistical Mechanics of Rigid Spheres", J. Chem. Phys. 31 369 (1959).
5. Helfand, E. and Frisch, H.L. "Theory of Two- and One-dimensional Rigid Sphere Fluids", J. Chem. Phys. 34 1037 (1961).
6. Edwards, J.C. and Chaiken, R.F. "Detonation Calculations with a Percus-Yevick Equation of State", U.S. Bureau of Mines, RI 7905, 1974.
7. Ree, F.H. and Hoover, W.G. "Seventh Virial Coefficients for Hard-spheres and Hard Disks", J. Chem. Phys. 46 4181 (1967).
8. Carnahan, N.F. and Starling, K.E. "Equation of State for Nonattracting Rigid Spheres", J. Chem. Phys. 51 635 (1969).
9. Guggenheim, E.A. "Variations on van der Waals Equation of State for High Densities" Mol. Phy. 9 199 (1965).
10. Thiele, E.T. "Equation of State for Hard-spheres", J. Chem. Phys. 39 474 (1963).
11. Scott, R.L. "Physical Chemistry an advanced treatise", Vol VIII A, Henderson, D., Ed., Chapter 1, 1971.

12. Mohan, V.K. and Hay, J.E. "Reparameterization of the Becker-Kistiakowsky - Wilson Equation of State for Water-Gel Explosives", Combustion and Flame 50 207 (1983).

13. Hornig, H.C., Lee, E.L. and Finger, M. "Equation of State of Detonation Products", Proceedings of the Fifth Symposium (International) on Detonation, Office of Naval Research, p. 503, 1970.

14. Dremin, A.N. and Shvedow, K.K. Zh. Prikl. Mekh. Tekn. Fiz., 3 154 (1964) (Translation).

15. Fickett, W. "Detonation Properties of Condensed Explosives Calculated with an Equation of State Based on Intermolecular Potentials", Los Alamos Scientific Laboratory Report LA-2712 (1962).

16. Lee, E.L. and Hornig, H.C. "Equation of State of Detonation Product Gases", Twelfth Symposium (International) on Combustion, p. 493 (1969).

17. Apin, Y.A. and Voskoboynikov, I.M., HMFT, p. 117 (1961).

18. Gibson, F.C., Bowser, M.L., Summers, C.R., Scott, F.H. and Mason, C.M. "Use of an Electro-optical Method to Determine Detonation Temperature in High Explosives", J. Applied Phys. 29 628 (1958).

19. Van Dolah, R.W., Gibson, F.C. and Murphy, J.N. "Sympathetic Detonation of Ammonium Nitrate-fuel Oil", Bureau of Mines RI-6746, 1966.

20. Van Dolah, R.W., Gibson, F.C. and Murphy, J.N. "Further Studies on Sympathetic Detonation", Bureau of Mines RI-6903, 1966.

21. Chaiken, R.F., Cook, E.B. and T.C. Rube "Toxic Fumes from Explosives: Ammonium Nitrate - Fuel Oil Mixtures", U.S. Bureau of Mines, RI 7867, 1974.

22. Johansson, C.H. and Persson, P.A. "Detonics of High Explosives", p. 39, Academic Press, New York, 1970.

Table 1. Comparison of calculated and experimental detonation products (moles/kg explosive) for two ANFO mixtures (density = 0.8 gm/cm^3)

Explosive	Product	Experimental values [21]		Calculated [20]			This work CS
		Crawshaw Jones	Large Gallery	Modified BKW	Virial	JCZ 3	(λ=0.35)
1 ANFO (94/6)	CO_2	2.6667	4.70	3.6185	3.530	3.8447	3.7747
	CO	0.6994	0.3888	0.6739	0.761	0.4476	0.5177
	NO	0.0003	0.0535	0.0039	0.053	0.0038	0.0271
2 ANFO (97/3)	CO	2.4166	0.222	0.0003	0.002	0.0002	0.0009
	NO	0.6388	0.583	0.1717	0.888	0.2291	0.4067
	O_2	0.0	2.555	2.7795	2.400	2.7507	2.6599

Table 2. Comparison of calculated detonation temperatures for two liquid explosives

Explosive	Initial density (gm/cm^3)	Detonation Temperature, K				
		Experimental			Calculated	
		U.S. Bu Mines	Los Alamos	Gibson et al.	CS	JCZ 2
NG	1.60	4025	3470	3896 4095 4079	5065	4540
NM	1.30	3800	3750		3751	3482

Explosive	Detonation Temperature, K				
	Calculated				
	JCZ 3	BRL	Cook	Mader	BKW
NG	4528	5073	6170	3216	3068
NM	3558	3962	--	3120	2559

Table 3. Calculated results for isopropylnitrate (ρ = 1.137 g/cm^3)

	CS	BKW	MBKW
P(atm)	27970	85607	49484
T(k)	1403	937	1332
D(m/s)	3357	5792	4227
CO (mole/kg explosive)	0.7530	0.0	0.2248
NO (mole/kg explosive)	0.0	0.0	0.0
Total gas (mole/kg explosive)	36.39	35.28	35.74

TABLE 4

ELEMENTAL COMPOSITION OF THE AMMONIUM NITRATE-LOADED SLURRY EXPLOSIVES INVESTIGATED

Table to be inserted

(Direction of EMR due to confidentiality of its contents)

Table 5. Comparison of calculated C-J state and detonation products (NO and CO) for ammonium nitrate-loaded slurry explosives

	CALCULATED VALUES											
	CS						MBKW					
Slurry explosive	P(atm)	D(m/sec)	T(k)	NO (mol/kg explosive)	CO (mol/kg explosive)	Total gas (mol/kg explosive)	P(atm)	D(m/sec)	T(k)	NO (mol/kg)	CO (mol/kg)	Total gas (mol/kg)
1	73991	4603	2467	0.0	1.3331	37.83	126317	5870	2283	0.0	1.4871	35.95
2	54841	4545	3777	0.1363	0.6720	37.02	75780	4998	3383	0.0257	0.9135	36.93
3	47415	4243	2605	0.2430	0.0048	39.25	72914	4903	2298	0.0	0.0019	39.06
4	89961	5184	3031	0.0208	0.5360	38.40	111357	5534	2355	0.0	0.9492	37.94
5	56992	4511	3473	0.0143	-	36.17	83786	5165	3129	0.0018	0.0	35.83
6	44943	3585	3043	0.2914	0.0276	32.30	-	-	-	-	-	-
7	46230	3532	3020	0.3873	0.0172	32.49	-	-	-	-	-	-
8	58996	4250	3685	0.0881	0.5639	29.51	95119	5239	3474	0.0279	0.7810	28.09
9	27598	3227	2387	0.1927	0.0008	34.20	-	-	-	-	-	-
10	42871	3724	3593	0.1542	0.3280	29.40	69630	4691	3470	0.0759	0.4002	29.42
11	55780	4220	2703	0.0	1.7096	35.77	-	-	-	-	-	-
12	45552	3883	2040	0.0	0.4463	37.81	-	-	-	-	-	-

Table 5. (cont'd)

	BKW						PYC (λ=0.372)					
Slurry explosive	P(atm)	D(m/sec)	T(k)	NO (mol/kg explosive)	CO (mol/kg explosive)	Total gas (mol/kg explosive)	P(atm)	D(m/sec)	T(k)	NO (mol/kg)	CO (mol/kg)	Total gas (mol/kg)
1	-	-	-	-	-	-	-	-	-	-	-	-
2	108667	6167	2814	0.0013	0.8575	36.64	58440	4784	3787	0.1336	0.6639	37.01
3	113118	6315	1687	0.0	0.0033	38.58	47366	4207	2597	0.2452	0.0045	40.59
4	173322	7184	1451	0.0	0.0267	36.97	82709	5397	2876	0.0070	0.7562	38.83
5	120988	6398	2622	0.0	-	34.54	60643	4737	3482	0.0141	-	36.11
6	-	-	-	-	-	-	-	-	-	-	-	-
7	-	-	-	-	-	-	-	-	-	-	-	-
8	-	-	-	-	-	-	-	-	-	-	-	-
9	-	-	-	-	-	-	-	-	-	-	-	-
10	-	-	-	-	-	-	-	-	-	-	-	-
11	-	-	-	-	-	-	70863	4849	3478	0.0712	0.4588	33.64
12	-	-	-	-	-	-	-	-	-	-	-	-

Table 6. The calculated constant volume explosion state for ammonium nitrate-loaded slurry explosives

Slurry explosive	P(atm)	V(cc/gm)	T(k)
2	26384	0.9434	3448
5	27470	0.8647	3182

Table 7. The calculated Hugoniot curve for ammonium nitrate-loaded slurry explosive #2

P(atm)	V(cc/gm)	T(k)
49996	0.7270	3720
40025	0.7896	3603
30054	0.8894	3489
20082	1.0773	3378
10110	1.5978	3270

Table 8. The calculated isolines for ammonium nitrate-loaded slurry explosive #2 at two conditions

V(cc/gm)	P(atm)	T(k)	P(atm)	V(cc/gm)	T(k)
0.94	39999	4870	50000	0.9401	5696
	38999	4778		0.9359	5668
	37996	4684		0.9318	5637
	36997	4589		0.9278	5607
	35998	4492		0.9238	5576
	34998	4392		0.9198	5546
	33999	4290		0.9158	5515
	32999	4186		0.9118	5483
	32000	4079		0.9078	5452
	31000	3969		0.9038	5420
	30000	3856		0.8998	5388

Table 9. The calculated Hugoniot curve for ammonium nitrate-loaded slurry explosive #5

P(atm)	V(cc/gm)	T(k)
49997	0.6823	3402
44886	0.7090	3551
39775	0.7419	3301
34664	0.7833	3251
29553	0.8375	3202
24442	0.9120	3154
19331	1.0224	3108
14220	1.2056	3063
9109	1.5799	3021
3997	2.8594	2981

Table 10. The calculated isolines for ammonium nitrate-loaded slurry explosive #5 at two conditions

V(cc/gm)	P(atm)	T(k)	P(atm)	V(cc/gm)	T(k)
0.7500	50019	4204	50000	0.7501	4204
	47999	4048		0.7450	4146
	46002	3889		0.7400	4087
	43997	3727		0.7350	4028
	42002	3565		0.7300	3969
	40002	3400		0.7250	3909
	38001	3234		0.7200	3850
	36000	3068		0.7150	3790
	34000	2902		0.7100	3731
	32000	2736		0.7050	3671
	29999	2569		0.7000	3612

Table 11. The calculated C-J state and detonation products (NO and CO) for ammonium nitrated-loaded slurry explosive #2 with various amount of aluminum

Al (% by mass)	P(atm)	D(m/sec)	T(k)	NO (mol/kg explosive)	CO (mol/kg explosive)	Total gas (mol/kg explosive)
1.10	47587	4285	2765	0.5949	0.0039	42.51
2.18	49110	4343	2916	0.6374	0.0079	41.74
3.24	50458	4393	3063	0.6481	0.0155	41.00
4.27	51656	4438	3204	0.6209	0.0292	40.29
5.29	52737	4477	3339	0.5511	0.0550	39.60
6.28	53698	4518	3463	0.4403	0.1055	38.95
7.25	54517	4545	3570	0.3151	0.2018	38.38
8.20	54729	4548	3652	0.2201	0.3478	37.88
9.13	54817	4547	3718	0.1664	0.5126	37.44
10.04	54841	4545	3777	0.1363	0.6720	37.02

Table 12. The calculated C-J state and detonation products (NO and CO) for ammonium nitrated-loaded slurry explosive #3 with various amount of $NaNO_3$

$NaNO_3$ (% by mass)	P(atm)	D(m/sec)	T(k)	NO (mol/kg explosive)	CO (mol/kg explosive)	Total gas (mol/kg explosive)
11.59	57527	4618	2735	0.0020	1.0915	43.26
22.50	47415	4243	2605	0.2430	0.0048	39.25

Table 13. The calculated C-J state and detonation products (NO and CO) for ammonium nitrate-loaded slurry explosive #10 with various amount of $Ca(NO_3)_2$

$Ca(NO_3)_2$ (% by mass)	P(atm)	D(m/sec)	T(k)	NO (mol/kg explosive)	CO (mol/kg explosive)	Total gas (mol/kg explosive)
16.36	47460	3974	3586	0.0271	1.2046	31.29
20.68	44604	3819	3602	0.0652	0.6860	30.09
23.30	42871	3724	3593	0.1542	0.3280	29.40

Table 14. The calculated C-J state and detonation products (NO and CO) for ammonium nitrate-loaded slurry explosive #10 with various amount of $NaNO_3$

$NaNO_3$ (% by mass)	P(atm)	D(m/sec)	T(k)	NO (mol/kg explosive)	CO (mol/kg explosive)	Total gas (mol/kg explosive)
0.52	44826	3830	3617	0.0609	0.7512	30.02
3.54	43350	3749	3604	0.1182	0.4265	29.46
4.02	43112	3737	3599	0.1348	0.3758	29.46
6.60	41637	3659	3546	0.2698	0.1690	29.17

Table 15. The calculated C-J state and detonation products (NO and CO) for ammonium nitrate-loaded slurry explosive #10 with various amount of aluminum

Al (% by mass)	P(atm)	D(m/sec)	T(k)	NO (mol/kg explosive)	CO (mol/kg explosive)	Total gas (mol/kg explosive)
1.15	32463	3438	1908	0.1211	0.0	35.83
4.44	44366	3680	2458	0.3617	0.0006	34.01
13.90	42871	3724	3593	0.1542	0.3280	29.40

Table 16. The calculated C-J state and detonation products (NO and CO) for ammonium nitrate-loaded slurry explosive #10 with silicon replacing aluminum

Si (% by mass)	P(atm)	D(m/sec)	T(k)	NO (mol/kg explosive)	CO (mol/kg explosive)	Total gas (mol/kg explosive)
1.15	33208	3482	1917	0.1235	0.0	36.15
10.41	51615	4165	3360	0.2091	0.1138	34.36
12.23	54611	4295	3539	0.0583	0.5936	34.20
13.90	57025	4396	3659	0.0370	1.0191	34.16

Table 17. The calculated C-J state and detonation products (NO and CO) for ammonium nitrate-loaded slurry explosive #10 with various amount of $NaNO_3$ and $Ca(NO_3)_2$

$NaNO_3$ (% by mass)	$Ca(NO_3)_2$ (% by mass)	P (atm)	D (m/sec)	T (k)	NO (mol/kg explosive)	CO (mol/kg explosive)	Total gas (mol/kg explosive)
12.8	15.00	43191	3743	3565	0.1309	0.3474	29.84
22.8	5.00	43565	3765	3530	0.1060	0.3740	30.38
23.3	4.50	43583	3767	3528	0.1049	0.3754	30.41
26.8	1.00	43706	3774	3516	0.0971	0.3855	30.59

Table 18. The calculated C-J state and detonation products (NO and CO) for ammonium nitrate-loaded slurry explosive #9 with various amount of inert added

Inert	Inert (% by mass)	P (atm)	D (m/sec)	T (k)	NO (mol/kg explosive)	CO (mol/kg explosive)	Total gas (mol/kg explosive)
Na_2O	3.85	27191	3204	2441	0.2026	0.0010	32.89
	4.76	27084	3198	2454	0.2048	0.0011	32.58
	5.66	26977	3192	2466	0.2070	0.0012	32.28
CaO	1.07	27976	3241	2444	0.2108	0.0010	33.84
	2.12	28344	3253	2499	0.2289	0.0014	33.50
	4.76	29291	3279	2639	0.2765	0.0027	32.66
	9.09	30931	3306	2865	0.3574	0.0071	31.35
SiO_2	0.99	28417	3264	2458	0.2168	0.0011	34.04
	4.76	32050	3386	2727	0.3180	0.0039	33.55
	9.09	39772	3482	2994	0.4376	0.0098	33.49
$CaCO_3$	1.07	27546	3217	2419	0.2013	0.0009	33.84
	4.76	27353	3179	2529	0.2318	0.0017	32.60

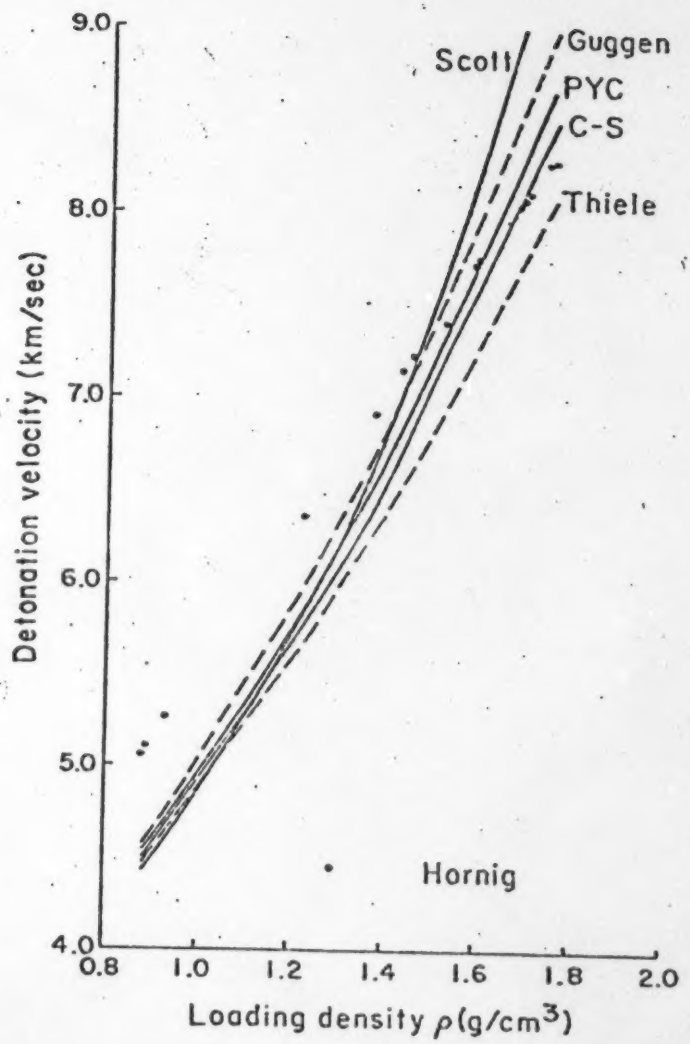

Figure 1 - Comparison of experimental C-J detonation velocities for PETN with calculated values from hard-sphere equations

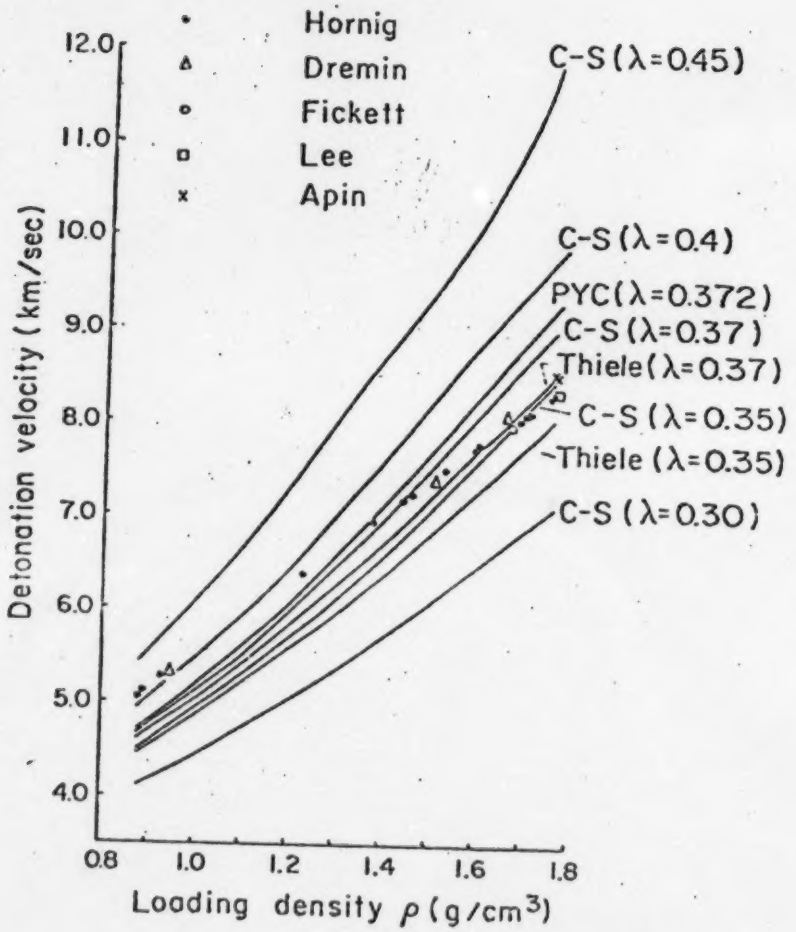

Figure 2 - Effect of the adjustable parameter λ

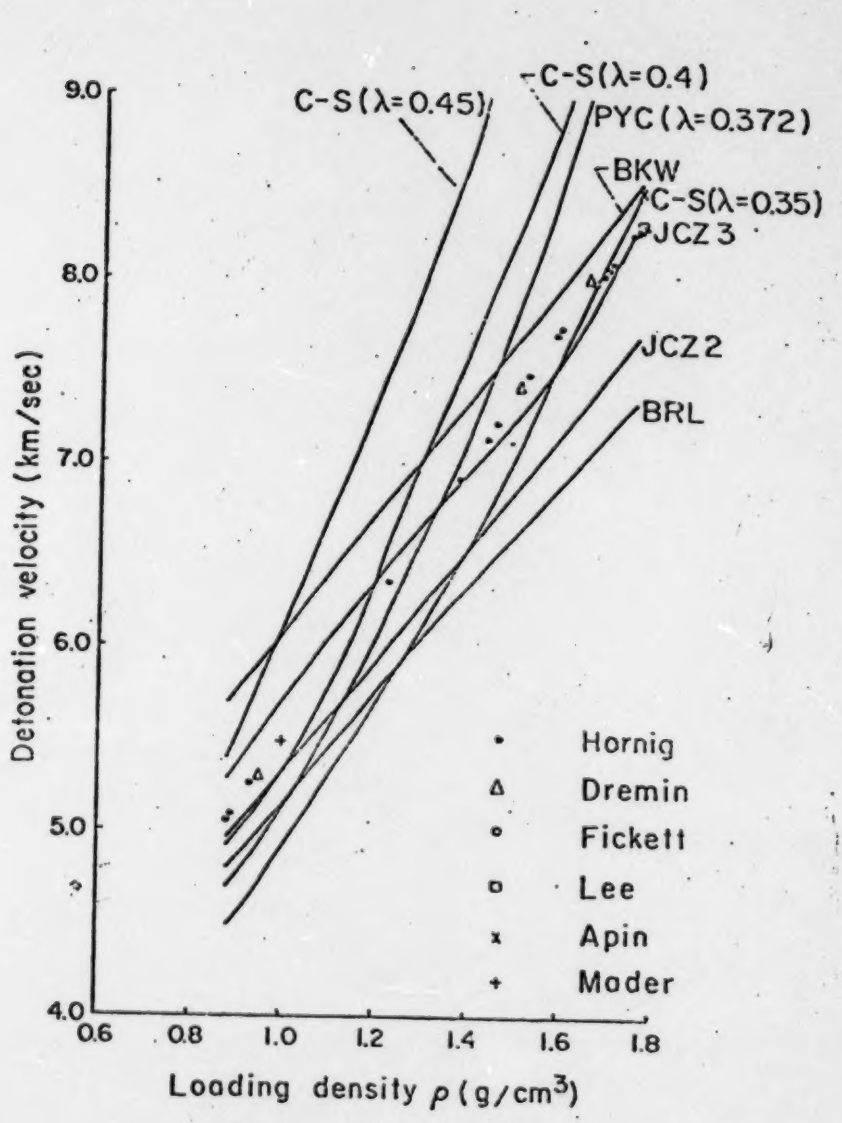

Figure 3 - Comparison of calculated and experimental C-J detonation velocities for PETN

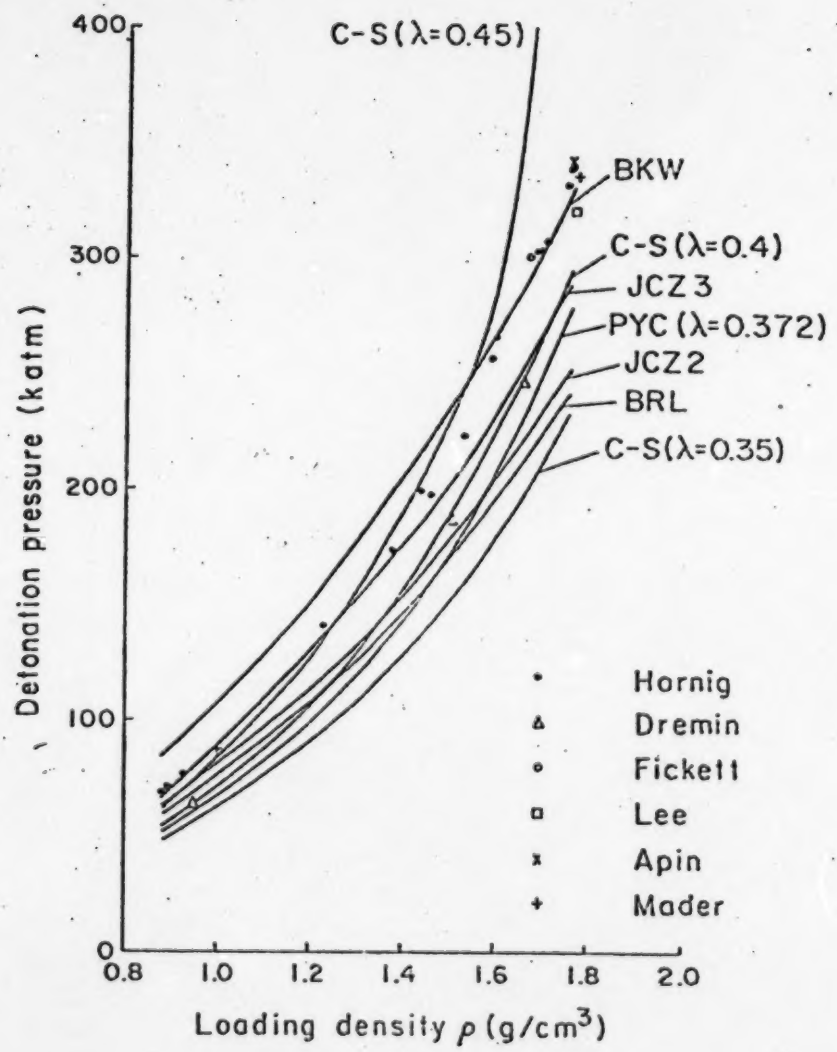

Figure 4 - Comparison of calculated and experimental C-J detonation pressures for PETN

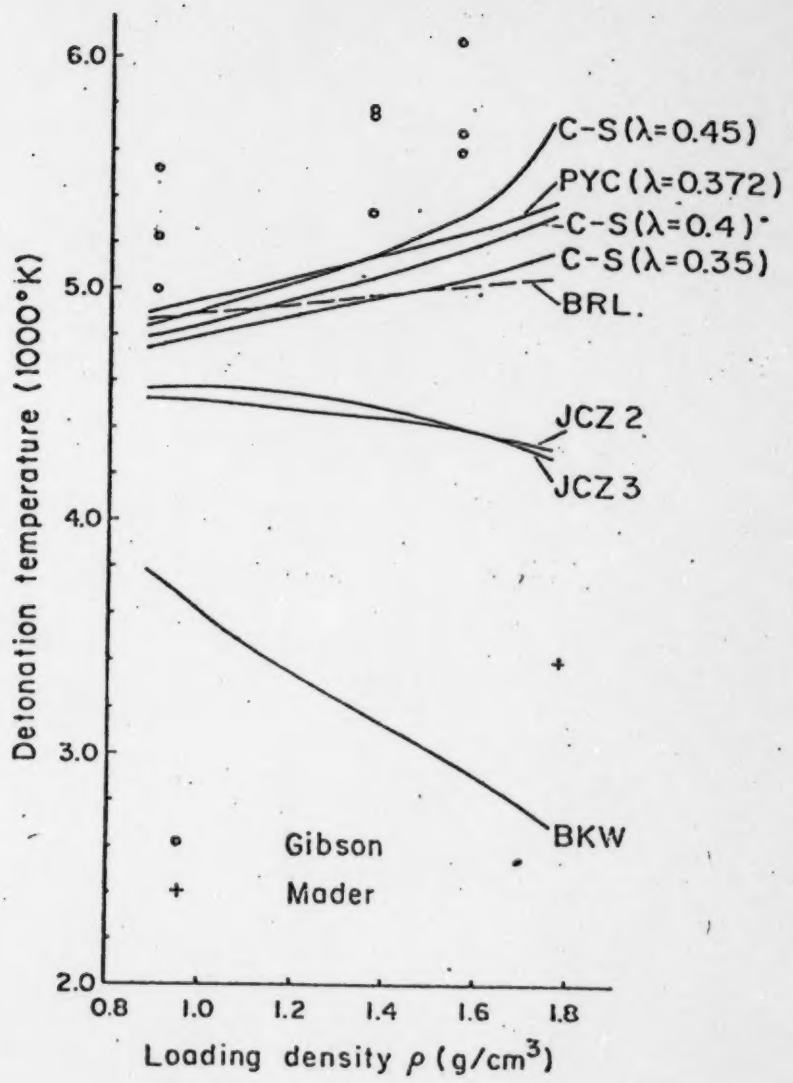

Figure 5 - Comparison of calculated and experimental C-J detonation temperatures for PETN

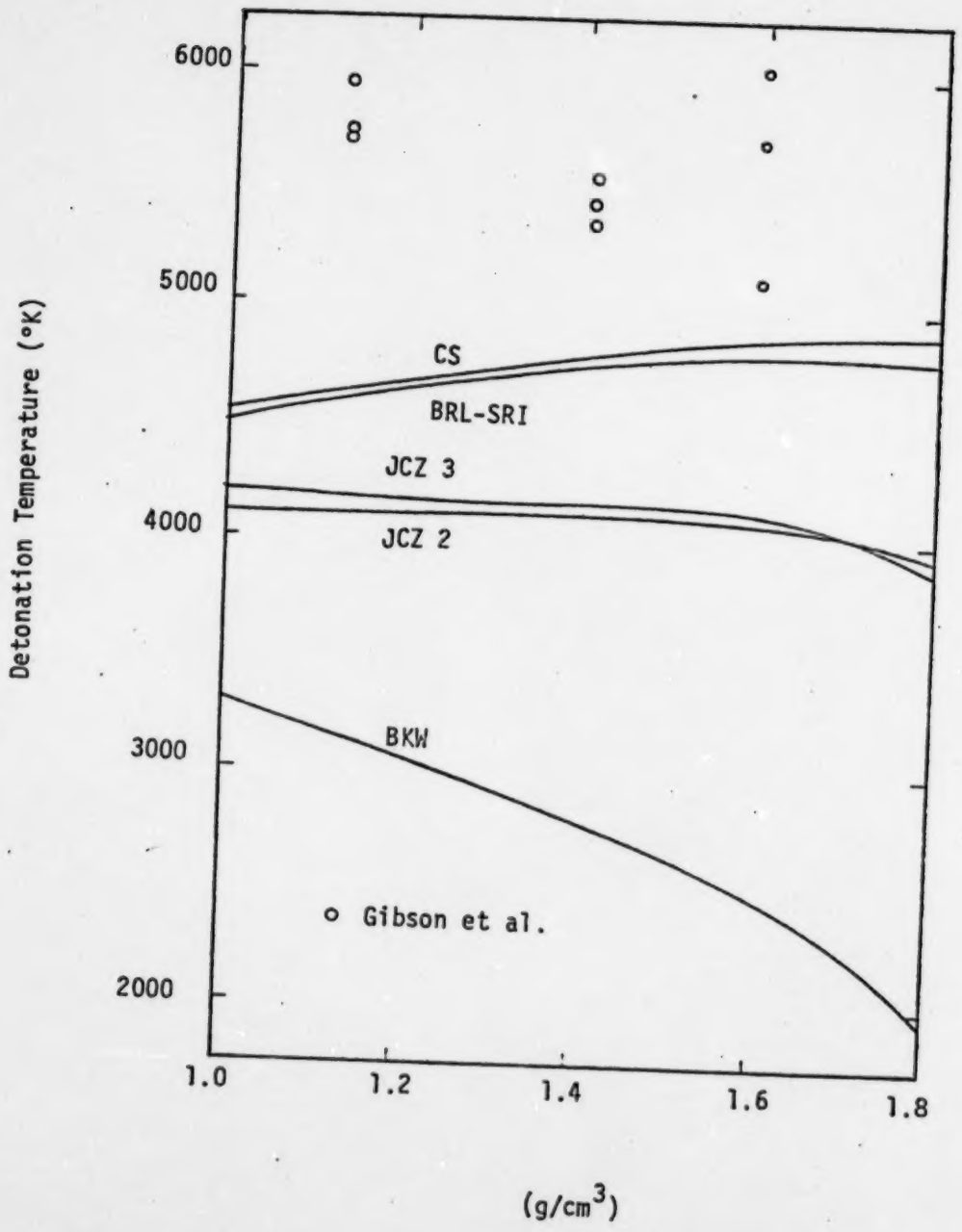

Figure 6. Comparison of calculated detonation temperature for RDX

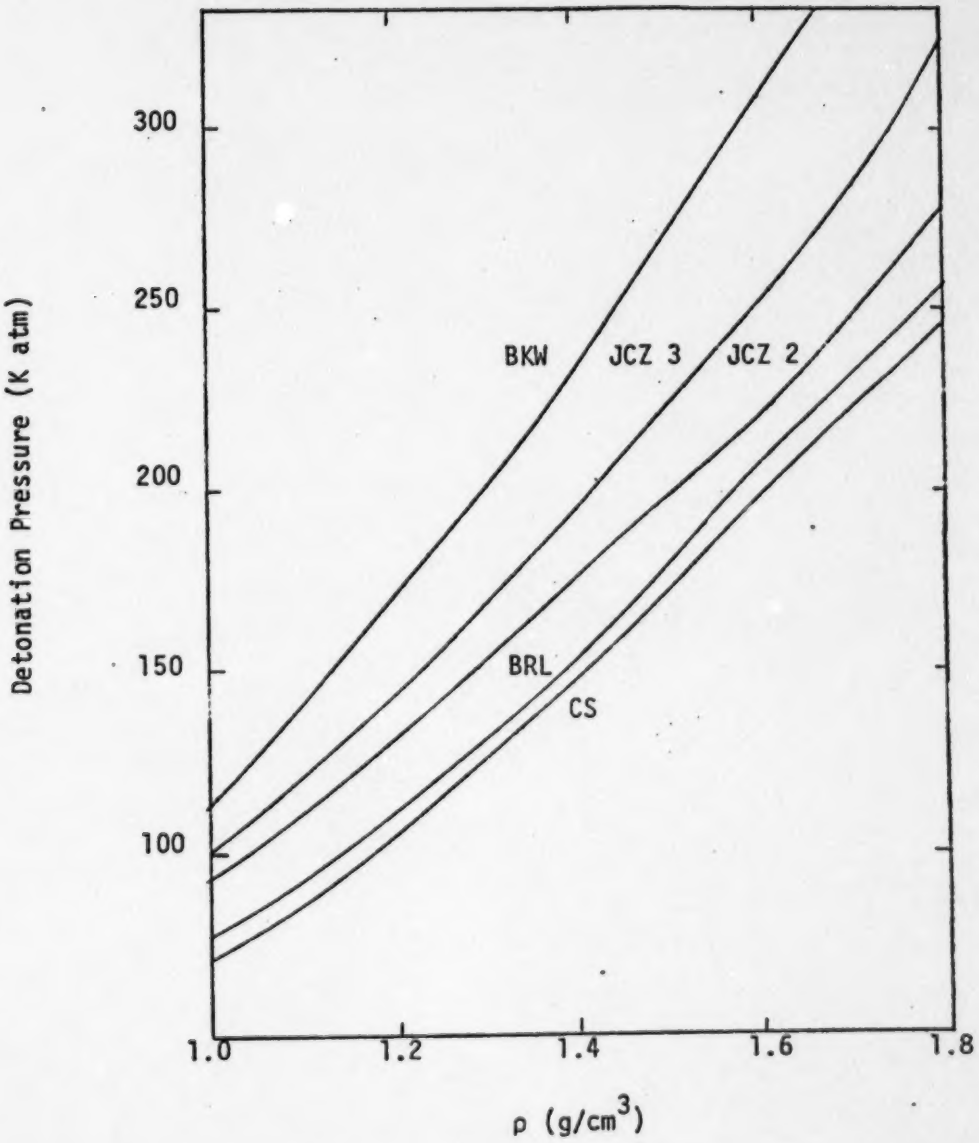

Figure 7. Comparison of calculated detonation pressure for RDX

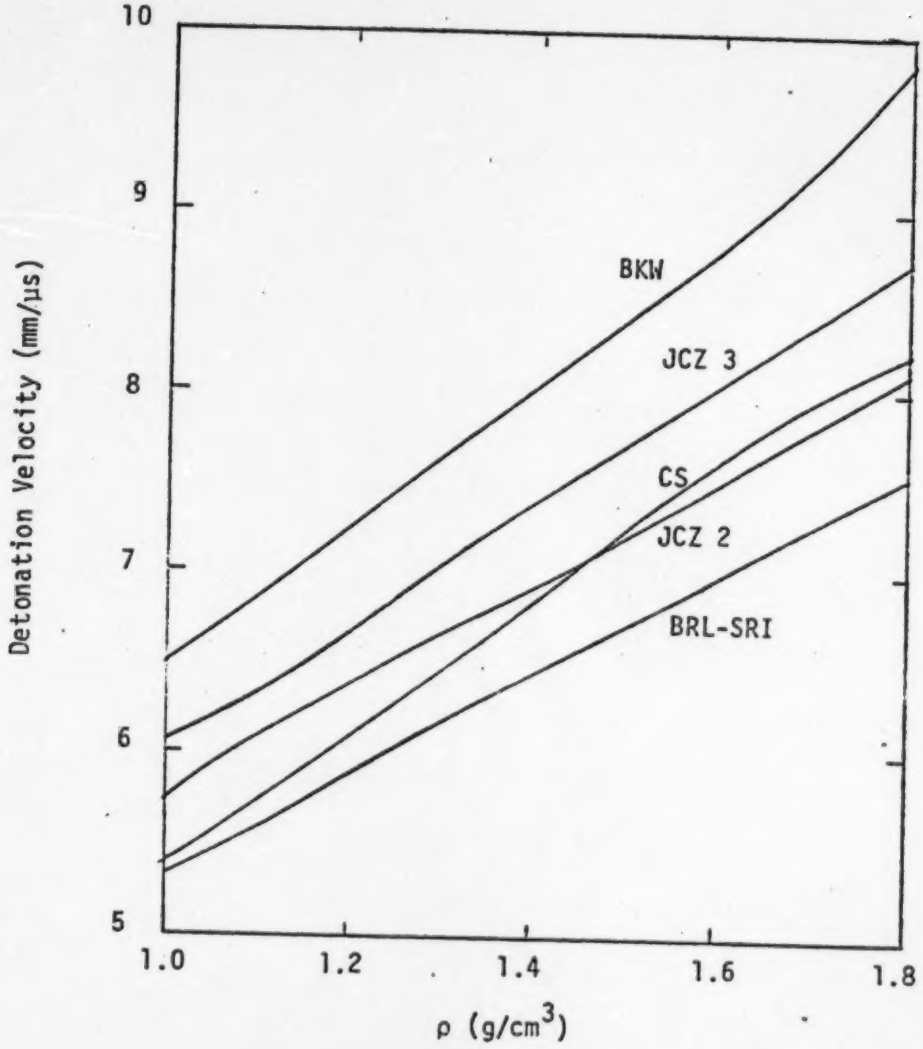

Figure 8. Comparison of calculated detonation velocities for RDX

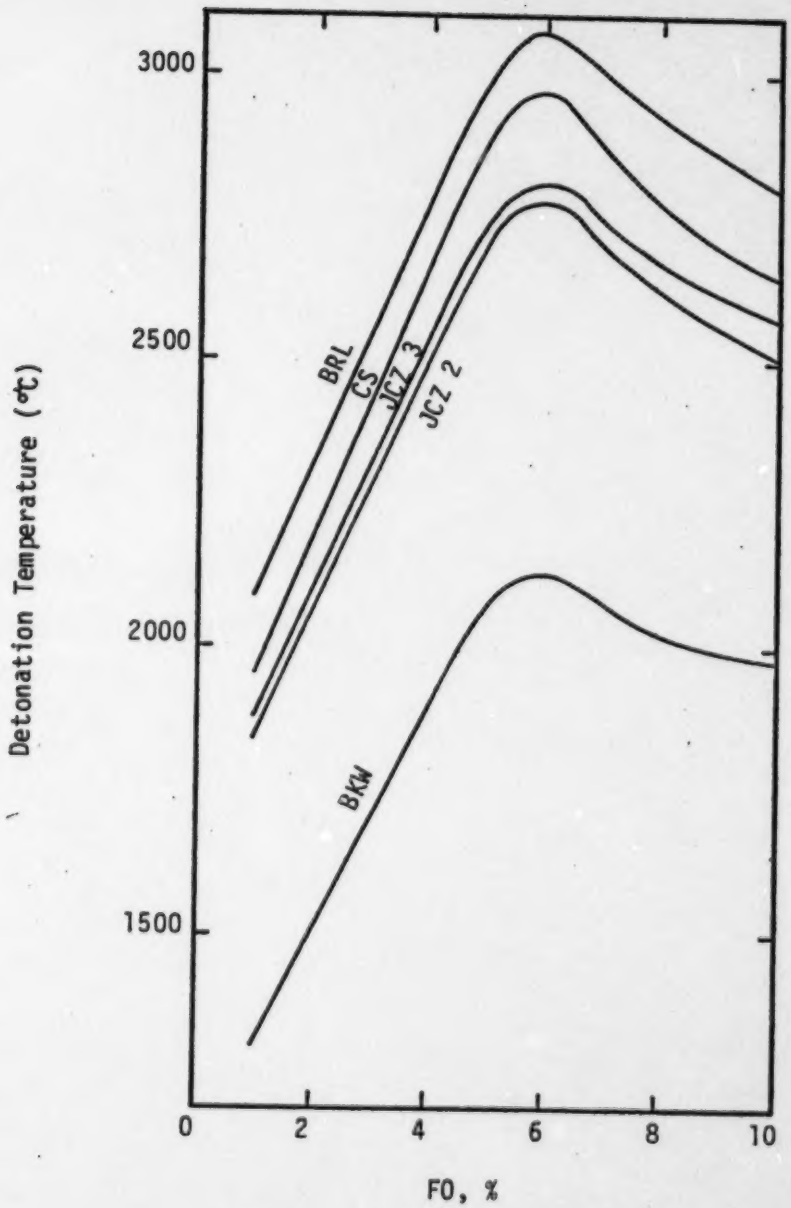

Figure 9. Comparison of calculated temperature for ANFO. $\rho = 0.8$ (g/cm^3), AN : NH_4NO_3, FO : $C_{7.17}H_{14}$

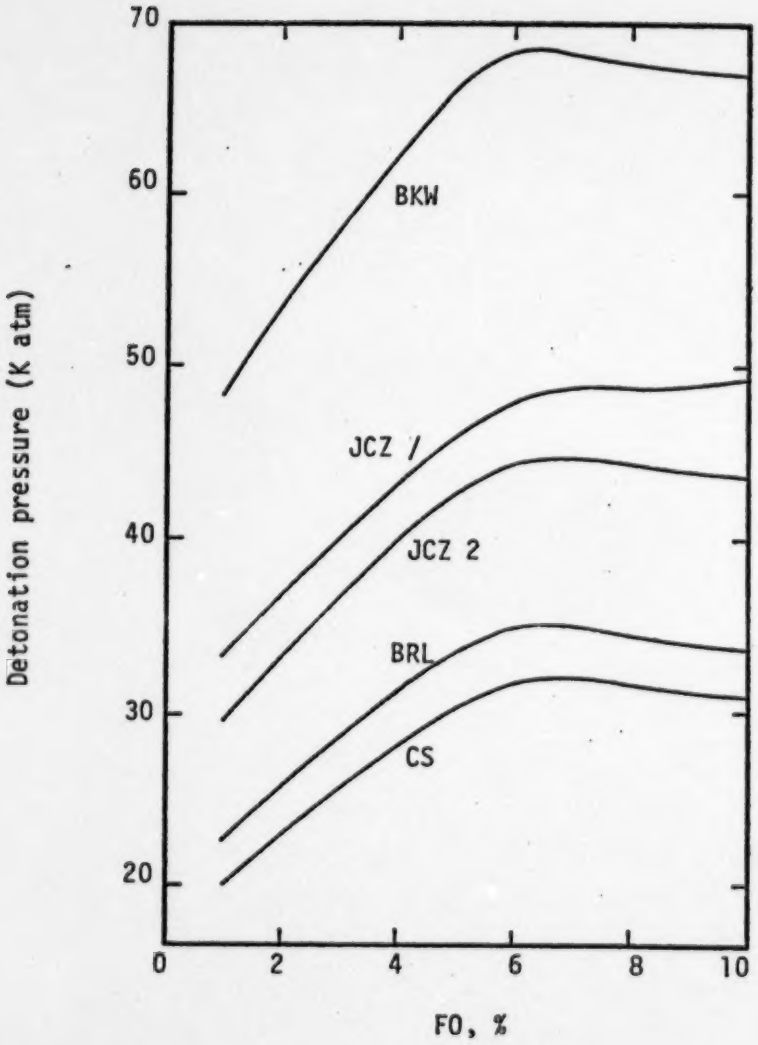

Figure 10. Comparison of calculated pressure for ANFO. $\rho = 0.8$ (g/cm^3), AN : NH_4NO_3, FO: $C_{7.17}\ H_{14}$

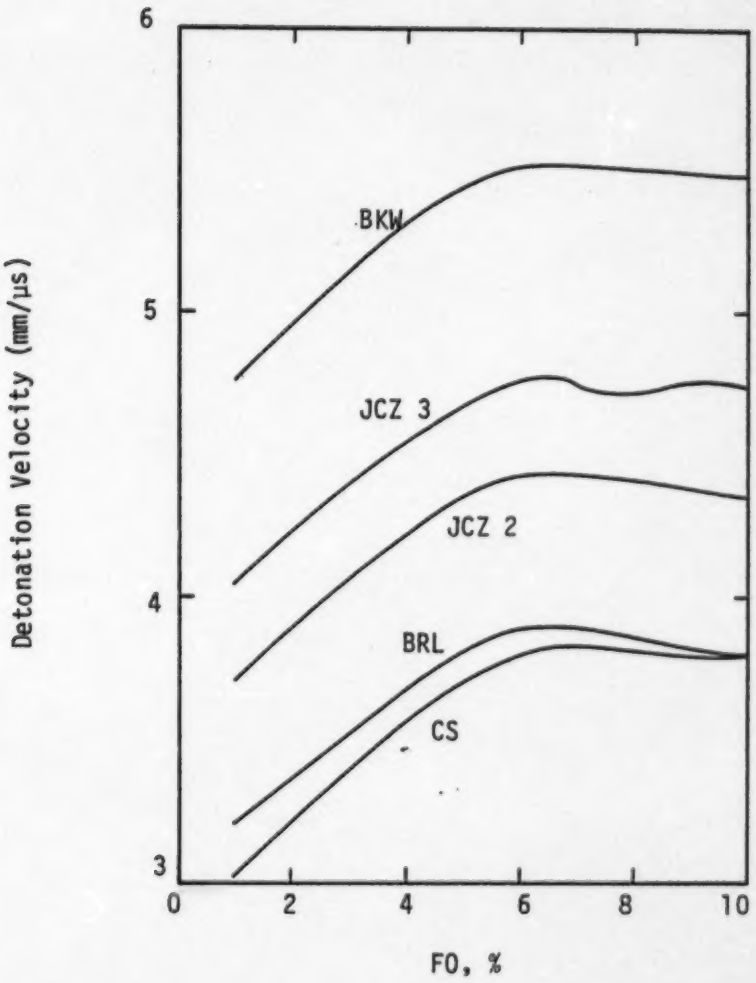

Figure 11. Comparison of calculated detonation velocities for ANFO. $\rho = 0.8$ (g/cm^3), AN : NH_4NO_3, FO : $C_{7.17}H_{14}$

APPENDIX

COMPUTER PROGRAM FOR SUBROUTINE EOS (LANE)

```
      SUBROUTINE HS1EOS(LANE)                                                  FENG
      COMMON   / TIGER / ADEXP, AJSJ, NOCTS, ALPHA, NTOC, BETA, BIG, BJSJ FENG
     A, CHIJSJ, CPHI, CPJSJ, CV, E0, E, EOF, EPETA1, EPETA2, EPETA3, EPE FENG
     ATA4, EPS, EPSPSI, EPSPT, EPST, FL, G, H0, H, HCON, HETAT1, HETAT2, FENG
     A IBUG, ICE, IDEAL, IERROR, ITC1L, ITC2L, ITC3L, ITC4L, ITOP, JUMP, FENG
     A KILL, KPRINT, LI, LIB, LINCT, LO, MAXCHO, MAXFOR, MAXORD, MAXPT,   FENG
     AMAXREJ, MIXED, NCC1, NCC, NCG, NCMSV, NCT1, NCT2, NCT, NEQ, NNIS,   FENG
     ANOALF, NOCASE, NOCHO, NOFLT, NOFORM, NOORD, NOREJ, NOTOT, NPAGE, N FENG
     APTSV, NSC, NSF, NSFF, NSG, NSM, NST, NSTOR, P0, P, KGEOS, PCON, PE FENG
     ATAT1, PETAT2, PHIJSJ, PHIRHO, PHIT, PSIZ, PSIZZ, R, RHO0, RHO, RX,  FENG
     A S0, S, SX, T0, T, TACON, ZNAME, TINITL, TMCON, TSAVE, UMJSJ, V0,   FENG
     AV, VCON, VETAT1, VETAT2, WCHI, WCP, WM, WMU, WP, XN, XUM1, XUM2      FENG
     A , NOGEOS                                                            FENG
      COMMON   / TIGRE / AJS(40), BJS(40), BG(40), CHII(40), CHIJS(40), C FENG
     AN(40), CHO(40), CPI(40), CPJS(40), ELM(40), ETA(15), ETETA1(15), F FENG
     A(40), FLTA(50), GAMMA(40), GAMRHO(40), GAMT(40), GETA(15), HETA(15 FENG
     A), IC(80), IXCC(40), IXCT(40), IXMC(40), KIND(40), KX(40), ORD(40) FENG
     A, PETA(15), PHIJS(40), PHIN(40), PSI(40), Q(40), QA(40), REJ(40),   FENG
     ASG(40), UMI(40), UMJS(40), VETA(15), W(40),          WT(40), X(40),  FENG
     A XETAT1(40), XETAT2(40), XNAME(40), Y(40), ZC(80), ZCX(80), TYP(80 FENG
     A), VAL(80), ZCC(80), NOGC(40)                                        FENG
      COMMON   / TYGER / A(40, 15), AL(15, 3, 3), AS(15, 3, 3), B(40, 15) FENG
     A, CC(40, 15), CG(40, 9), CL(15, 9), CNETA(15, 15), CS(15, 9), D(40 FENG
     A, 40), FORM(15,20), STORNI(50, 15), STOR(15, 33), SVP(147, 4), TEM FENG
     AA(15, 20)                                                            FENG
       DIMENSION SKI(85),DBDN(85,85),SKII(85),AA(85),DBDTHS(85)
     * ,DBDT2(85),WK(85),ZNMSV(85)
      NOEOS -- EQUATION OF STATE NUMBER = 1   FRISCH
                                        = 2   SCOTT 2
                                        = 3   GUGGEN
                                        = 4   THIELE
                                        = 5   SCOTT 1
                                        = 6   VDW
                                        = 7   HS C-S
      GO TO (10,10,10,10,120,130,140,160,250,270,290,300,320,330), LANE

         INITIAL CALCULATION

   10 CONTINUE
      RGAS = 82.05606/WM                                                    TEST
      DBDT = 0.0
      DBDTH2 = 0.0
       DO 500 I = 1, NSG
      DBDTHS(I) = 0.0
      DBDT2(I) = 0.0
      DBDT = X(I)*DBDTHS(I) + DBDT
      DBDTH2 = X(I)*DBDT2(I) + DBDTH2
  500 CONTINUE
      SK = 0.0
      DO 20       I = 1, NSG
      SKI(I) = 0.0                                                          CUBIC M-
      DO 20 J = 1, NSG
      SKI(I) = SKI(I) +X(J)*((WK(I)+WK(J))/2.)**3                           CUBIC MR
   20 SK = SK + X(I)*X(J)*((WK(I)+WK(J))/2.)**3
      DO 8181 I = 1, NSG                                                    CUBIC MR
      SKII(I) =0.0                                                          CUBIC MR
      DO 8181 J = 1, NSG                                                    CUBIC MR
      SKII(I) = SKII(I) +X(J)*((WK(I)+WK(J))/2.0)**3                        CUBIC MR
 8181 CONTINUE
      DO 8182 I = 1, NSG                                                    CUBIC MR
      DO 8182 J = 1, NSG                                                    CUBIC MR
      DBDN(I,J) = 2.*(((WK(I)+WK(J))/2.0)**3+1.*SK-SKII(I)-1.*SKII(J) )     CUBIC MR
 8182 CONTINUE                                                              CUBIC MR
      DO 8888 I = 1, NSG                                                    CUBIC MR
       AA(I) =SKI(I)*2.0 - SK                                               CUBIC MR
 8888 CONTINUE                                                              CUBIC M-
```

```
      YHS = 3.1416/6.*6.022045E23*RHO*SK*XLAMDA/WM
      IF ( LANE - 2) 50, 50, 80

         LANE 1 AND 2 CALCULATION

   50 CONTINUE
      GO TO (1,2,3,4,5,6,7), NOEOS
    1 CONTINUE
      CPHI = (1.+YHS + YHS**2)/(1.-YHS)**3                                  FRISCH
      GO TO 19
    2 CONTINUE
      CPHI = (1.+3.*YHS+4.*YHS**2)/(1.-2.*YHS)/(1.+YHS)                     SCOTT-2
      GO TO 19
    3 CONTINUE
      CPHI = 1.     /(1.-YHS)**4                                            GUGGEN.
      GO TO 19
    4 CONTINUE
      CPHI = (1.+2.*YHS+3.*YHS**2)/(1.-YHS)**2                              THIELS
      GO TO 19
    5 CONTINUE
      CPHI = (1.+2.*YHS)/(1.-2.*YHS)                                        SCOTT-1
      GO TO 19
    6 CONTINUE
      CPHI = 1./(1.-4.*YHS)                                                 VDW
      GO TO 19
    7 CONTINUE
      CPHI =(1.+YHS + YHS**2-YHS**3)/(1.-YHS)**3                            HS C-S
      GO TO 19
   19 CONTINUE
      GO TO (21,22,23,24,25,26,27), NOEOS
   21 CONTINUE
      PHIRHO = YHS*(1.+2.*YHS)/(1.+YHS+YHS**2) + 3.*YHS/(1.-YHS)            FRIS38
      GO TO 39
   22 CONTINUE
      PHIRHO = YHS*(3.+8.*YHS)/(1.+3.*YHS+4.*YHS**2)+YHS*(1.+4.*YHS)/       SCOTT-2
     * (1.-2.*YHS)/(1.+YHS)                                                 SCOTT-2
      GO TO 39
   23 CONTINUE
      PHIRHO = 4.*YHS/(1.-YHS)                                              GUGGSN8C
      GO TO 39
   24 CONTINUE
      PHIRHO = 2.*YHS*(1.+3.*YHS)/(1.+2.*YHS+3.*YHS**2)+2.*YHS/(1.-YHS)     THIELE
      GO TO 39
   25 CONTINUE
      PHIRHO = 4.*YHS/(1.+2.*YHS)/(1.-2.*YHS)                               SCOTT- 1
      GO TO 39
   26 CONTINUE
      PHIRHO = 4.*YHS/(1.-4.*YHS)                                           VDW
      GO TO 39
   27 CONTINUE
      PHIRHO = YHS*(1.+3.*YHS)*(1.-YHS)/(1.+YHS+YHS**2-YHS**3) + 3.*YHS/HS C-20
     * (1.-YHS)                                                            HS C-S
      GO TO 39
   39 CONTINUE
      GO TO (41,42,43,44,45,46,47), NOEOS
   41 CONTINUE
      PHIT = T*DBDT/SK*PHIRHO                                               FRISCH
      GO TO 59
   42 CONTINUE
      PHIT = T*DBDT/SK*PHIRHO                                               SCOTT- 2
      GO TO 59
   43 CONTINUE
      PHIT = T*DBDT/SK*PHIRHO                                               GUGGEN.
      GO TO 59
   44 CONTINUE
      PHIT = T*DBDT/SK*PHIRHO                                               THIELE
```

```
      GO TO 59
   45 CONTINUE
      PHIT = T*DBDT/SK*PHIRHO                                          SCOTT-1
      GO TO 59
   46 CONTINUE
      PHIT = T*DBDT/SK*PHIPHO                                          VDW
      GO TO 59
   47 CONTINUE
      PHIT = T*DBDT/SK*PHIRHO                                          HS 3--S
      GO TO 59
   59 CONTINUE
      IF (LANE - 2) 350, 60, 350

         LANE 2 CALCULATIONS

   60 CONTINUE
      DO 70 I = 1, NSG
      GO TO (61,62,63,64,65,66,67), NOEOS
   61 CONTINUE
      PHIN(I) = AA(I)/SK*PHIRHO                                        FRISCH
      GO TO 79
   62 CONTINUE
      PHIN(I) = AA(I)/SK*PHIRHO                                        SCOTT-2
      GO TO 79
   63 CONTINUE
      PHIN(I) = AA(I)/SK*PHIRHO                                        GUGGEN.
      GO TO 79
   64 CONTINUE
      PHIN(I) = AA(I)/SK*PHIRHO                                        THIELE
      GO TO 79
   65 CONTINUE
      PHIN(I) = AA(I)/SK*PHIRHO                                        SCOTT-1
      GO TO 79
   66 CONTINUE
      PHIN(I) = AA(I)/SK*PHIRHO                                        VDW
      GO TO 79
   67 CONTINUE
      PHIN(I) = AA(I)/SK*PHIRHO                                        HS C-S
      GO TO 79
   79 CONTINUE
      GO TO (81,82,83,84,85,86,87), NOEOS
   81 CONTINUE
      GAMRHO(I) = YHS*((4.-2.*YHS+YHS**2)/(1.-YHS)**3+AA(I)/SK*SX      FRISCH
     *   *(2.+YHS)**2/(1.-YHS)**4)                                     FRISCH
      GO TO 99
   82 CONTINUE
      GAMRHO(I) =2.*YHS/3.*(3.*(2.+3.*YHS)/(1.-2.*YHS)/(1.+YHS)        SCOTT-2
     * +    AA(I)/SK*SX*(7./(1.-2.*YHS)**2+1./(1.+YHS)**2))           SCOTT-2
      GO TO 99
   83 CONTINUE
      GAMRHO(I) = YHS*(4.-6.*YHS+4.*YHS**2-YHS**3)/(1.-YHS)**4 + AA(I) GUGG5 N.
     *   /SK*SX*YHS/(1.-YHS)**5*4.0                                    GUGG5N C
      GO TO 99
   84 CONTINUE
      GAMRHO(I) = 2.*YHS*(3.*SK/SX-4.*AA(I))/SK*SX/(1.-YHS)**2         THIELE
     * -2.*YHS/(1.-YHS)+12.*YHS*AA(I)/SK*SX/(1.-YHS)**3                THIELE
      GO TO 99
   85 CONTINUE
      GAMRHO(I) = 4.*YHS/(1.-2.*YHS)+4.*AA(I)*YHS/SK*SX/(1.-2.*YHS)**2 SCOTT-1
      GO TO 99
   86 CONTINUE
      GAMRHO(I) = 4.*YHS/(1.-4.*YHS)*(1.+AA(I)/SK*SX/(1.-4.*YHS))      VDW
      GO TO 99
   87 CONTINUE
      GAMRHO(I) = YHS*(2.*(2.-YHS)/(1.-YHS)**3+2.*AA(I)/(SK/SX)*       HS C-S
     *   (2.+2.*YHS-YHS**2)/(1.-YHS)**4)                               HS 3-2
      GO TO 99
   99 CONTINUE
```

```
      GO TO (101,102,103,104,105,106,107), NOEOS
  101 CONTINUE
      GAMT(I) = T*YHS*(4.-2.*YHS+YHS**2)*DBDT/SK/(1.-YHS)**3                FRISCH
     *  +T*(4.*YHS-2.*YHS**2+YHS**3)/SK*SX/(1.-YHS)**3*DBDTHS(I)           FRISCH
     *  +T*AA(I)*YHS**2*(10.-2.*YHS+YHS**2)*DBDT/SK/SK*SX/(1.-YHS)**4      FRISCH
      GO TO 119
  102 CONTINUE
      GAMT(I) = 2.*T*YHS*DBDT/3./SK/SK*SX*(3.*(2.+3.*YHS)/(1.-2.*YHS)*    SCOTT-2
     * SK/SX/(1.+YHS)+AA(I)*( 7./(1.-2.*YHS)**2+1./(1.+YHS)**2-(8.+5.*    SCOTT-2
     * YHS)/(1.-2.*YHS)/(1.+YHS)))+2.*T*YHS*(8.+5.*YHS)*DBDTHS(I)/3./SK   SCOTT-2
     * *SX/(1.+YHS)/(1.-2.*YHS)                                            SCOTT-2
      GO TO 119
  103 CONTINUE
      GAMT(I) = T*YHS*DBDT*(4.-6.*YHS+4.*YHS**2-YHS**3)/SK/(1.-YHS)**4    GUGGEN.
     * +YHS*DBDTHS(I)/SK*SX/(1.-YHS)**4*(4.-6.*YHS+4.*YHS**2-YHS**3)       GUGGEN.
     * +AA(I)*YHS**2*(10.-10.*YHS+5.*YHS**2-YHS**3)*DBDT/SK/SK*SX/         GUGGEN.
     * (1.-YHS)**5                                                         GUGGEN.
      GO TO 119
  104 CONTINUE
      GAMT(I) = 2.*T*((SK/SX*DBDTHS(I)-AA(I)*DBDT/SX)+SK/SX*((3.-2.*YHS)  THIELE
     * *DBDT/SX-4.*DBDTHS(I))/(1.-YHS)-(3.*SK/SX-4.*AA(I))*(1.-2.*YHS)     THIELE
     **DBDT/SX/(1.-YHS)**2+3.*SK/SX*DBDTHS(I)/(1.-YHS)**2-3.*AA(I)        THIEL 5
     * *(1.-3.*YHS)*DBDT/SX/(1.-YHS)**3)                                  THIELE
      GO TO 119
  105 CONTINUE
      GAMT(I) = 4.*T*YHS*DBDT/SK/(1.-2.*YHS)+4.*T*YHS*DBDTHS(I)/SK*SX     SCOTT-1
     * /(1.-2.*YHS)+8.*T*AA(I)*YHS**2*DBDT/SK/SK*SX/(1.-2.*YHS)**2        SCOTT-1
      GO TO 119
  106 CONTINUE
      GAMT(I) = 4.*T*YHS*DBDT/SK/(1.-4.*YHS)+4.*T*YHS*(SK*DBDTHS(I)        VDW
     * +AA(I)*DBDT)/SK/SK*SX/(1.-4.*YHS)-4.*AA(I)*T*YHS*DBDT*(1.-8.*YHS)   VDW
     * /SK/SK*SX/(1.-4.*YHS)**2                                             VDW
      GO TO 119
  107 CONTINUE
      GAMT(I) =T*YHS/SK*DBDT*2.*(2.-YHS)/(1.-YHS)**3+2.*YHS*(2.-YHS)*T*   HS 3C-S
     *  DBDTHS(I)/(SK/SX)/(1.-YHS)**3+2.*AA(I)*YHS**2*T*DBDT*(5.-2.*YHS)HS C-S
     *  /(SK*SK/SX)/(1.-YHS)**4                                           HS 3-20
      GO TO 119
  119 CONTINUE
   70 CONTINUE
      GO TO (121,122,123,124,125,126,127), NOEOS
  121 CONTINUE
      EPS = -SX*T*DBDT*YHS*(4.-2.*YHS+YHS**2)/SK/(1.-YHS)**3                FRISCH
      GO TO 139
  122 CONTINUE
      EPS = -2.*SX*T/SK*SX*(2.+3.*YHS)/(1.-2.*YHS)/(1.+YHS)                 SCOTT-2
      GO TO 139
  123 CONTINUE
      EPS=-T*DBDT/SK*SX*(4.*YHS-6.*YHS**2+4.*YHS**3-YHS**4)/(1.-YHS)**4 GUGGEN.
      GO TO 139
  124 CONTINUE
      EPS = -2.*SX*T*YHS*(2.+YHS)*DBDT/SK/(1.-YHS)**2                       THIELE
      GO TO 139
  125 CONTINUE
      EPS = -4.*SX*T*YHS*DBDT/SK/(1.-2.*YHS)                                SCOTT-1
      GO TO 139
  126 CONTINUE
      EPS = -4.*T*SX*YHS*DBDT/SK/(1.-4.*YHS)                                 VDW
      GO TO 139
  127 CONTINUE
      EPS = SX*T*DBDT/SK*2.*YHS*(2.-YHS)/(1.-YHS)**3                        8S 3 2
      GO TO 139
  139 CONTINUE
      IF (YHS .GE. 1.0) GO TO 159
      GO TO (141,142,143,144,145,146,147), NOEOS
  141 CONTINUE
      EPSPT = -SX*T*(2.*DBDT+T*DBDTH2)*(4.-2.*YHS+YHS**2)/SK/(1.-YHS)**3 FRISCH
     * *YHS-SX*T*T*YHS**2*DBDT**2/SK/SK*(10.-2.*YHS+YHS**2)/(1.-YHS)**4 FRISCH
```

```
      GO TO 159
  142 CONTINUE
      IF (YHS .GE. 0.5) GO TO 159
      EPSPT = -SX*T/SK*((2.*DBDT+T*DBDTH2)*(-7./3.*ALOG(1.-2.*YHS)          SCOTT-2
     * -5./3.*ALOG(1.+YHS))+ 8.*T*DBDT**2/3./SK*(-.5*ALOG(1.-2.*YHS)        SCOTT-2
     *-ALOG(1.+YHS)) +2.*T*DBDT**2/SK*(11./3.*ALOG(1.-2.*YHS)+13./3.        SCOTT-2
     **ALOG(1.+YHS)+7./3.*2.*YHS/(1.-2.*YHS)-5./3.*YHS/(1.+YHS))            SCOTT-2
     * +(DBDT + DBDTH2)*(7./3.*ALOG(1.-2.*YHS)+5./3.*ALOG(1.+YHS)+7./3.    SCOTT-2
     * *2.*YHS/(1.-2.*YHS)-2./3.*YHS/(1.+YHS))+T/27.*DBDT**2/SK*(-218.      SCOTT-2
     **ALOG(1.-2.*YHS)-294.*2.*YHS/(1.-2.*YHS)+63.*(4.*YHS-4.*YHS**2)       SCOTT-2
     * /(1.-2.*YHS)**2-214.*ALOG(1.+YHS)+150.*YHS/(1.+YHS)-18.*(2.*YHS      SCOTT-2
     * +YHS**2)/(1.+YHS)**2)+4.*T/SK*DBDT**2*(26./27.*ALOG(1.-2.*YHS)       SCOTT-2
     * +13./27.*ALOG(1.+YHS)+7./9.*2.*YHS/(1.-2.*YHS)-2./9.*YHS/(1.+YHS     SCOTT-2
     * ))                                                                   SCOTT-2
      GO TO 159
  143 CONTINUE
      EPSPT = -SX*T/SK/(1.-YHS)**4*(2.*DBDT+T*DBDTH2)*(4.-6.*YHS+4.*YHS     GUGGEN.
     * **2-YHS**3)*YHS+SX*T*T*DBDT/SK/SK/(1.-YHS)**5*YHS**2*(10.-10.*YHS    GUGGEN
     * +5.*YHS**2-YHS**3)                                                   GUGGEN
      GO TO 159
  144 CONTINUE
      EPSPT = -SX*T*YHS/SK*SX/(1.-YHS)**2*((4.*DBDT/SX+2.*T*DBDTH2/SX)      THIELE
     * *(2.+YHS)+2.*YHS*(YHS+5.)*T*(DBDT/SX)**2/SK*SX/(1.-YHS))             THIELE
      GO TO 159
  145 CONTINUE
      EPSPT = -2.*SX*T/SK*(2.*DBDT+T*DBDTH2)*2.*YHS/(1.-2.*YHS)             SCOTT-1
     * -SX*T*T*DBDT**2/SK/SK*8.*YHS**2/(1.-2.*YHS)**2                       SCOTT-1
      GO TO 159
  146 CONTINUE
      EPSPT = -SX*T/SK*(2.*DBDT+T*DBDTH2)*4.*YHS/(1.-4.*YHS)                VDW
     * -SX*T*T*DBDT**2/SK/SK*16.*YHS**2/(1.-4.*YHS)**2                      VDW
      GO TO 159
  147 CONTINUE
      EPSPT = -2.*SX*SX*T/SK*(2.*DBDT/SX+T*DBDTH2/SX**2)*YHS*(2.-YHS)/      HS C-S
     *  (1.-YHS)**3-4.*T*T/SK/SK*SX**3*DBDT**2*YHS**2*(5.-2.*YHS)/2./       8S 3-S
     *   (1.-YHS)**4                                                        HS C-S
      GO TO 159
  159 CONTINUE
      GO TO 350
   80 DO 90 I = 1, NSG
       IF ( YHS .GE. 1.0) GO TO 179
      GO TO (161,162,163,164,165,166,167), NOEOS
  161 CONTINUE
      GAMMA(I) =3.*YHS*(2.-YHS)/2./(1.-YHS)**2-ALOG(1.-YHS)+AA(I)/SK*SX     FRISCH
     *  *YHS*(4.-2.*YHS+YHS**2)/(1.-YHS)**3                                 FRISCH
      GO TO 179
  162 CONTINUE
      IF (YHS .GE. 0.5) GO TO 179
      GAMMA(I) = -7./3.*ALOG(1.-2.*YHS)-2./3.*ALOG(1.+YHS)+2.*AA(I)*YHS     SCOTT-2
     * /3./SK*SX*(7./(1.-2.*YHS)+1./(1.+YHS))                              SCOTT-2
      GO TO 179
  163 CONTINUE
      GAMMA(I) = (18.*YHS-27.*YHS**2+11.*YHS**3)/6./(1.-YHS)**3-ALOG(1.     GUGGEN.
     * -YHS)+AA(I)/SK*SX*YHS/(1.-YHS)**4*(4.-6.*YHS+4.*YHS**2-YHS**3)       GUGGENC
      GO TO 179
  164 CONTINUE
      GAMMA(I) = 2.*(3.*SK/SX-4.*AA(I))/SK*SX/(1.-YHS)+2.*ALOG(1.-YHS)      THIELE
     * +6.*AA(I)/SK*SX/(1.-YHS)**2-2.*(3.-AA(I)/SK*SX)                      THIELE
      GO TO 179
  165 CONTINUE
       IF ( YHS .GE. 0.5) GO TO 179
      GAMMA(I) = -2.*ALOG(1.-2.*YHS)+4.*AA(I)*YHS/SK*SX/(1.-2.*YHS)         SCOTT-1
      GO TO 179
  166 CONTINUE
       IF ( YHS .GE. .25) GO TO 179
      GAMMA(I) = AA(I)*4.*YHS/SK*SX/(1.-4.*YHS)-ALOG(1.-4.*YHS)               VDW
      GO TO 179
  167 CONTINUE
```

```
      GAMMA(I) = YHS*(4.-3.*YHS)/(1.-YHS)**2+2.*AA(I)*YHS*(2.-YHS)/SK/   HS C-S
     *   (1.-YHS)**3*SX                                                   HS C-S
      GO TO 179
  179 CONTINUE
   90 CONTINUE
      IF (LANE - 4) 350, 100, 350

         LANE 4 CALCULATIONS

  100 DO 110 I = 1, NSG
      DO 110 J = 1, NSG
      GO TO (181,182,183,184,185,186,187), NOEOS
  181 CONTINUE
      D(I,J) = YHS*(4.-2.*YHS+YHS**2)*(AA(I)+AA(J))/SK/(1.-YHS)**3+AA(I) FRISCH
     *  *AA(J)*YHS**2*(10.-2.*YHS+YHS**2)/SK/SK*SX/(1.-YHS)**4           FRISCH
     * + YHS*(4.-2.*YHS+YHS**2)/SK/(1.-YHS)**3*DBDN(I,J)                 CUBIC MR
      GO TO 199
  182 CONTINUE
      D(I,J) = 2.*AA(J)*YHS/SK*(2.+3.*YHS)/(1.+YHS)/(1.-2.*YHS)+2.*AA(I)SCOTT-2
     * *AA(J)*YHS**2/3./SK/SK*SX*(14./(1.-2.*YHS)**2-1./(1.+YHS)**2)+2.* SCOTT-2
     *   AA(I)*YHS/SK/3.0*(8.+5.*YHS)/(1.-2.*YHS)/(1.+YHS)               SCOTT-2
     * + 2.*YHS*(8.+5.*YHS)/3./SK/(1.-2.*YHS)/(1.+YHS)*DBDN(I,J)         CUBIC MR
      GO TO 199
  183 CONTINUE
      D(I,J) = YHS*((4.-6.*YHS+4.*YHS**2-YHS**3)*(1.-YHS)*SK/SX*(AA(I)   GUGGEN.
     * +AA(J))+AA(I)*AA(J)*YHS*(10.-10.*YHS+5.*YHS**2-YHS**3))/SK/SK*SX GUGGEN.
     * /(1.-YHS)**5                                                     GUGGEN33
     * +YHS*(4.-6.*YHS+4.*YHS**2-YHS**3)/SK/(1.-YHS)**4*DBDN(I,J)       CUBIC MR
      GO TO 199
  184 CONTINUE
      D(I,J) = -2./SK/SK*SX*(AA(I)*(AA(J)-SK/SX)-SK/SX*(3.*AA(J)-3.*SK  THIELE
     * /SX-AA(J)*YHS)/(1.-YHS)+(3.*SK/SX-4.*AA(I))*((1.-YHS)*(AA(J)      THIELE
     * -SK/SX)-AA(J)*YHS)/(1.-YHS)**2 + 3.*AA(I)*((1.-YHS)*(AA(J)-SK/SX) THIELE
     * -2.*AA(J)*YHS)/(1.-YHS)**3)                                       THIELE
     * +(5./SK/(1.-YHS)**2+2./SK-8./SK/(1.-YHS))*DBDN(I,J)               CUBIC MM
      GO TO 199
  185 CONTINUE
      D(I,J) =(4.*SK/SX*YHS*(1.-2.*YHS)*(AA(I)+AA(J))+8.*AA(I)*AA(J)     SCOTT-1
     * *YHS**2)/SK/SK*SX/(1.-2.*YHS)**2                                  SCOTT-1
     * + 4.*YHS/SK/(1.-2.*YHS)*DBDN(I,J)
      GO TO 199
  186 CONTINUE
      D(I,J) = 4.*AA(J)*YHS/SK/(1.-4.*YHS)+4.*AA(I)*AA(J)*YHS/SK/SK*SX   VDW
     * /(1.-4.*YHS)+4.*AA(I)*YHS*(4.*AA(J)*YHS+(1.-4.*YHS)*(SK/SX-AA(J)) VDW
     * ))/SK/SK*SX/(1.-4.*YHS)**2                                        VDW
     * + 4.*YHS/(1.-4.*YHS)/SK*DBDN(I,J)
      GO TO 199
  187 CONTINUE
      D(I,J) = 2.*YHS/SK**2/(1.-YHS)**4*(SK*(2.-YHS)*(1.-YHS)*(AA(I)+AA HS C-S
     *   (J))+SX*AA(I)*AA(J)*YHS*(5.-2.*YHS))                           HS 3 -0
     * + 2.*YHS*(2.-YHS)/SK/(1.-YHS)**3*DBDN(I,J)                       CUBIC MR
      GO TO 199
  199 CONTINUE
  110 CONTINUE
      GO TO 350

         LANE 5

  120 CONTINUE
      XLAMDA = 0.35
      NOEOS  = 7
      GO TO 350

         LANE 6

  130 NOCTS = 1
      NOSRD = 0
      GO TO 350
```

```
        LANE 7

140 IF(VAL(1) - 223301.0) 350,150,350
150 KGEOS = IDEAL
    GO TO 350
160 CONTINUE
    IF (VAL(1) - 223301.0) 350,351,350
351 IF(VAL(2) - 382615.0) 353,352,353
352 XLAMDA = VAL(3)
    GO TO 350
353 IF(VAL(2) - 282919.0) 350,354,350
354 NOEOS = VAL(3) + .5
    GO TO 350
250 CONTINUE
    IF (VAL(1) - 223301.0) 350, 261, 350
261 NOSRD = NOSRD + 1
    IF (NOSRD - 85)  262, 262, 264
262 ZNMSV(NOSRD) = VAL(2)
    WK(NOSRD) = VAL(3)
    GO TO 350
264 WRITE(LO, 266)
266 FORMAT(1H0,'******* ERROR TYPE 35 - TOO MANY HS1 CARDS')
    GO TO 350

        LANE 10

270 CONTINUE
    IF (NOSRD) 390, 390, 370
370 DO 380 I = 1, NOSRD
    IF (ZNAME - ZNMSV(I)) 380, 400, 380
380 CONTINUE
390 TYP(1) = 0.0
    GO TO 410
400 TYP(1) = WK(I)
410 IF (NOALF) 350,415,350
415 WRITE(LO, 280) TYP(1)
280 FORMAT(8X,'HS1   SIGMA      ',E14.6)
    GO TO 350

        LANE 11

290 WK(NOALF) = TYP(1)
    GO TO 350

        LANE 12

300 WRITE(LO,310) WK(NOALF)
310 FORMAT(14X,'HS1   SIGMA      ', E14.7)
    GO TO 350

        LANE 13

320 TYP(1) = WK(NOALF)
    GO TO 350

        LANE 14

330 WRITE(LO,340) NOEOS,XLAMDA
340 FORMAT(1H0,' HARD SPHERE EQUATION OF STATE - NOEOS = ',I5,' LAMDA
   *=    ' ,F10.7)
350 CONTINUE
    RETURN
    END
```